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Thermodynamic Properties of
Selected Minerals in the System
 $\text{Al}_2\text{O}_3\text{-CaO-SiO}_2\text{-H}_2\text{O}$
at 298.15 K and 1 Bar (10^5 Pascals)
Pressure and at Higher Temperatures

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By B. S. HEMINGWAY, J. L. HAAS, JR., and G. R. ROBINSON, JR.

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*A summary of thermodynamic data for
minerals in the system*

*$\text{Al}_2\text{O}_3\text{-CaO-SiO}_2\text{-H}_2\text{O}$ and tabulated
values for the functions $C_{p,T}^\circ$,*

$(H_T^\circ - H_{298}^\circ)/T$, S_T° , $(G_T^\circ - H_{298}^\circ)/T$,

*$\Delta H_{f,T}^\circ$, and $\Delta G_{f,T}^\circ$ at 298.15 K and at
temperatures as high as 1800 K. This*

*report is a supplement to U.S. Geological
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THERMODYNAMIC PROPERTIES OF SELECTED MINERALS IN THE SYSTEM Al₂O₃-CaO-SiO₂-H₂O at 298.15 K AND 1 BAR (10⁵ PASCALS) PRESSURE AND AT HIGHER TEMPERATURES

By B. S. HEMINGWAY, J. L. HAAS, JR., and G. R. ROBINSON, JR.

ABSTRACT

Tables of thermodynamic properties are presented for 7 oxide and hydroxide phases, for 7 aluminosilicate and hydrous aluminosilicate phases, and for 12 calcium silicate, calcium aluminosilicate, and hydrous calcium aluminosilicate phases.

Tabulated thermodynamic properties of selected phases from the system alumina-lime-silica-water have been calculated by the method described by J. L. Haas, Jr., and J. R. Fisher in 1976 from the compilation of experimental data described by Haas and others in 1981. The results presented here supersede the tabulated data for the same phases given by Robie and others in 1979.

In general, the data presented here are consistent with those given by Robie and others in 1979 but are not in agreement with the enthalpies and free energies of formation (elements) given by Helgeson and others in 1978 for aluminum-bearing phases. The addition of -6.5 kJ per mole of aluminum to the enthalpy and free-energy values of the aluminum-bearing phases (except gibbsite) reported by Helgeson and others eliminates most of the discrepancy. The difference between the values of the thermodynamic properties reported by Helgeson and others and our values is a consequence of a redefinition of the aluminum reference state within the data set they considered.

INTRODUCTION

The experimental data on selected phases in the alumina-lime-silica-water system were evaluated by using the method of Haas and Fisher (1976). The data are presented here as revisions and additions to the tables of thermodynamic properties published by Robie and others (1979). These tables are based upon the same physical constants and atomic weights as those given by Robie and others, are presented in the same format, and use the same symbol notation (see tables 1 and 2 in Robie and others).

The goal of this study was to produce a set of thermodynamic properties at 298.15 K and 1 bar and at higher temperatures for selected phases in the alumina-lime-silica-water system that is consistent with thermodynamic theory, the observed properties of each phase, and the

observed phase relations among the phases. The experimental data analyzed in this study were obtained from a search of the literature through June 1979.

Summaries of the experimental data upon which the derived thermodynamic properties reported herein are based, the methods of data treatment, and the criteria for data rejection have been given by Haas and others (1980, 1981).

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REFERENCE DATA

All evaluations must accept some base values without question. In this study, as in the paper by Robie and others (1979), the properties of the elements Al, Ca, H₂, O₂, and Si and of the oxides corundum, lime, quartz, and water as given by the CODATA Task Group (1978), Hultgren and others (1973), Stull and Prophet (1971), Chase and others (1974, 1975), and Fisher and Zen (1971) were accepted values. The properties of the evaluated phases were determined relative to these reference values.

In the course of evaluating the data presented in this study, no inconsistencies were found within the reference values that would suggest that a reevaluation of any of the reference base was necessary. Small differences between the thermodynamic properties of the reference oxide phases reported here and those of Robie and others (1979) are largely the consequence of fitting the experimental data to different polynomial equations. Such differences are not statistically significant.

Several of the chemical compositions are represented by more than one crystal structure. Tables for the reference state of these polymorphs are provided for convenience, in addition to a table for the polymorphic form present at 298.15 K and 1 bar. The reference-state tables are labeled with either the chemical formula or the phase name followed by the label "-Reference."

**COMPARISON OF RECENT TABULATIONS OF
THERMODYNAMIC DATA FOR PHASES IN THE SYSTEM
ALUMINA-LIME-SILICA-WATER**

A BRIEF STATEMENT OF THE PROBLEMS

The importance of aluminum-bearing phases to geologic processes makes it imperative that differences among the current tabulations of thermodynamic data for the phases be clearly delineated. The major sources of tabulated thermodynamic data for phases of geologic interest in the system alumina-lime-silica-water are Wagman and others (1968), Robie and Waldbaum (1968), Naumov and others (1971), Helgeson and others (1978), Hemingway and Robie (1977), Robie and others (1978, 1979), and Haas and others (1979, 1980, 1981). The tabulations published prior to 1977 contain internal inconsistencies related to the use of $AlCl_3 \cdot 6H_2O$ and gibbsite as aluminum reference compounds (see Hemingway and Robie, 1977; Hemingway and others, 1978) and therefore will not be discussed further. The compilation by Robie and others (1979) supersedes the earlier tabulations by Robie and Waldbaum (1968) and Robie and others (1978). The data of Haas and others represent the same data set reported here with the exception that Haas and others (1980, 1981) reported their results for a standard reference pressure of 1 atmosphere.

The thermodynamic properties of the aluminum-bearing phases are referenced to the enthalpy and free energy of formation of gibbsite as reported by Hemingway and Robie (1977) for all tabulations except those of Haas and others (1979, 1980, 1981) and this study, where the secondary aluminum reference phase was corundum. In the work of Robie and others (1979), corundum is also used as the secondary aluminum reference phase for the higher temperature and (or) higher pressure reactions. The thermodynamic data for the two secondary aluminum reference phases may be compared through the series of calorimetric, phase-equilibrium and silica-solubility experiments examined by the several sources of the tabulations cited above (for example, Hemingway and others, 1978).

In general, the data presented in this report and by Haas and others (1979, 1980, 1981) are consistent with the results of Robie and others (1979); that is, the thermodynamic properties listed for a phase are equivalent within the limits of standard calculations of the uncertainties (see, for example, Robie and others, 1979). Exceptions to this statement are found in the data for gehlenite and Ca-Al pyroxene. The assignment of zero uncertainty (refer to the section on confidence limits) to the contribution of the reference oxides, as was done in this study and by Haas and others (1980, 1981) reduces the uncertainty in the thermodynamic properties calculated with respect to formation

from the elements to about one-half the value that would otherwise be obtained (for example, in Robie and others). The uncertainties given for silicate phases referenced to the oxides may be directly compared with uncertainties for these phases tabulated by Robie and others.

The absolute values selected for the enthalpies and free energies of formation of phases presented in this report and by Haas and others (1980, 1981), Hemingway and Robie (1977), and Robie and others (1979) are not consistent with the enthalpies and free energies of formation derived by Helgeson and others (1978) for the same phases (see table 1). However, when the enthalpies and free energies of formation given by Helgeson and others are corrected by the addition of -6.5 kJ per mole of aluminum in the phase, the resultant values are in good agreement at 298.15 K.

A BRIEF DESCRIPTION OF THE METHODS USED IN COMPILING AND EVALUATING DATA FOR SEVERAL RECENT TABULATIONS OF THERMODYNAMIC DATA

In this section, we provide a short description of the methods used by Robie and others (1979), Helgeson and others (1978), Haas and others (1981), and this study. Some of the strengths and weaknesses of each compilation are discussed.

The tabulation of thermodynamic properties of minerals and compounds published by Robie and others (1979) was a major revision of the earlier tabulation by Robie and Waldbaum (1968). The results compiled by Robie and others were based primarily upon calorimetric data for the enthalpy of formation, heat capacity, heat content, and entropy of the phases presented. Phase-equilibrium, electrochemical-cell, and other sources of thermodynamic data were used to supplement the calorimetric data.

The major advantages of the approach followed by Robie and others (1979) are that the calorimetric thermochemical cycles are, in general, straightforward and can be well characterized, the samples used in the reaction scheme may be fully characterized after they have been prepared for the experiments, the thermochemical properties of many phases in a chemical system may be evaluated directly from reactions involving a limited number of reference phases, and proper experimental design will result in a well-defined final state for each enthalpy-of-solution reaction used in the thermochemical cycle. The major disadvantage of the method used by Robie and others (1979) is that not all phases of geologic interest are soluble in the same solvent, and, because each calorimetric thermochemical cycle can stand alone, there is no need to establish a network of interrelated reactions through which erroneous enthalpy-of-solution values might be detected. In addition, any secondary reaction (for example, the formation of a gel during

a dissolution reaction) may produce an undefined final state in one or more of the steps in the thermochemical cycle.

Helgeson and others (1978) used a procedure that is nearly the antithesis of that followed by Robie and others (1979). The evaluated thermodynamic data set published by Helgeson and others is based primarily upon experimental data taken from phase-equilibrium experiments. Calorimetric data and experimental results from other thermochemical data were relegated to a secondary or supplemental role. Helgeson and others (1978) used regression analysis of multiple sets of phase-equilibrium data; small sets for data of related phases were fitted separately, and continuity between sets was attained by fixing the matrix of parameters for one phase for each element; that is, by assigning fixed values to secondary reference materials. The values assigned to the enthalpies and free energies of formation of the phases from the elements are tied directly to the values chosen for the secondary reference materials.

The tabulations of thermodynamic data published by Haas and others (1979, 1980, 1981) and given in this study are based upon multiple-regression analysis of thermochemical data taken from all experimental processes and fitted simultaneously. To the extent possible, the regression analysis is performed on the directly observed experimental data, thus reducing the possibility of introducing inconsistencies in the process of converting the data to entropy, enthalpy, and free-energy-of-formation values. For example, in the procedure used by Haas and others and in this study, the directly measured enthalpy-of-solution values, rather than the enthalpy-of-formation values, were used.

The strength of the regression-analysis approaches (Helgeson and others, 1978; Haas and others, 1979, 1980, 1981; this study) lies in the use of reaction networks in which several reactions involving the thermodynamic data for a phase must be satisfied simultaneously. The precision of the data and the probability that the value is accurate increase as the number of reactions that the value must simultaneously satisfy increases and as the number of different types of experimental procedures from which the value is derived increases. In general, differences between values derived from different experimental procedures represent systematic errors associated with one or more of the procedures.

Necessarily, as the reaction network becomes sparse, values obtained by the regression procedures become less precise and less accurate. In addition, to obtain meaningful fits to the observed data, discordant data must be removed from the total set of data before the final regression analysis is performed. The source of the error causing data to be discordant is not always clearly established. Therefore, discordance of a value is not sufficient proof that the data value removed is in error,

nor is concordance proof of accuracy of the values that are retained. When a reaction involving one of the secondary standards contains errant data, that error can be propagated throughout the reaction network by redefining the reference state of the major element from that represented by the secondary reference phase.

To provide an efficient tabulation of thermochemical data, the observed data (obtained from dissimilar experimental procedures) must be converted to a unique reference system. Robie and others (1979) chose to reference the enthalpies and free energies of formation of the phases they listed to the properties of the elements (and, for some phases, to certain oxides). This procedure provides a convenient source of thermodynamic data for calculations, but it does not provide a direct and true measure of the uncertainty of any specific reaction written with respect to data in the tabulation. To illustrate this point, we shall examine the enthalpy of the low albite–analbite transition at 298.15 K and 1 bar. From the difference in the enthalpies of formation (from the elements) of low albite and analbite given by Robie and others, we obtain 10.88 ± 4.99 kJ. The data used by Robie and others were reported by Waldbaum and Robie (1971). On the basis of the direct measurements of the enthalpies of solution of low albite and analbite in aqueous hydrofluoric acid, Waldbaum and Robie reported 10.88 ± 1.26 kJ for the enthalpy of transition. The additional uncertainty associated with the data given by Robie and others arises from the remaining part of the thermochemical cycles required to convert the enthalpies of solution of the two phases to enthalpies of formation from the elements. Therefore, if the uncertainty associated with a given reaction is critical to the discussion of the reaction, one who uses data from tabulations such as those of Robie and others must examine the original experimental data to calculate a rigorous uncertainty.

Helgeson and others (1978) did not give specific estimates of the uncertainty of the thermodynamic values they selected. They did provide a good discussion of the problems associated with assigning uncertainties to specific values selected by regression analysis and also provided general guidelines for estimating the uncertainties in the different data types. As in the situation described above, where estimates of the uncertainty are relevant to a discussion based upon results taken from the tabulation of Helgeson and others, the estimates must be made through an examination of the original experimental data.

Haas and others (1979, 1980, 1981) and this study list values for the uncertainties of selected thermodynamic properties of the phases at 298.15 K and at the standard pressures used in each study. Haas and others also listed uncertainties for the properties at higher temperatures. The uncertainty for a thermodynamic value given by Haas and others (1981) and in this study is calculated from the

variance-covariance matrix derived from the relationships among phases in the data set upon which the regression analysis was performed. Haas and others (1981) assigned zero uncertainty to the thermodynamic properties of the reference oxide phases (which are listed in the section on reference data), although we recognize that an uncertainty is associated with the thermodynamic values for these phases. This zero-uncertainty convention was followed here because the derived uncertainty more clearly reflects our knowledge of the relative uncertainties between phases, without the additional uncertainty that is traditionally introduced when the experimental data are reduced to a standard thermodynamic value for the purpose of tabulation. For example, the uncertainty assigned to the enthalpy of formation of kaolinite in this study and in those of Haas and others is ± 1.1 kJ; the enthalpy of formation is based upon the simultaneous fit to four reactions for which the experimental uncertainties range from ± 0.3 to ± 1.3 kJ.

The uncertainties for thermodynamic properties relative to the oxides or elements listed in the tables in this report and in the compilations of Haas and others (1979, 1980, 1981) are values calculated from the variance-covariance matrix from the data set of Haas and others (1981) and are not compatible with the uncertainties listed in most tabulations of thermodynamic data. Also, it should be stressed that the tabulated uncertainties listed in the tables for each phase cannot be combined to calculate the uncertainty in thermodynamic properties for reactions among phases.

DISCUSSION

Possibly the most common source of error leading to discordant experimental results is the systematic error; that is, any part of an experiment that produces a significant deviation of the result and goes undetected in the analysis of the experiment. In some cases, the errors arise from physical phenomena; in others, they arise from an incomplete analysis of the data or from incorrect assumptions regarding the data. Systematic errors manifest themselves as changes in the reference state of an element when they go undetected in an analysis of thermochemical data; they may affect the entire data base or only a part of it.

A detailed discussion of the types of systematic error that might occur in the several types of experimental procedures from which thermodynamic data are extracted is not appropriate in this discussion. However, one example will illustrate the problem. The enthalpy of formation from the elements of forsterite may be obtained by dissolving forsterite, periclase, and quartz in an appropriate solvent, measuring the enthalpies of solution of each phase, calculating the enthalpy of the

reaction of 2 periclase + quartz = forsterite, and adding the enthalpies of formation of 2 periclase and quartz. The enthalpy of formation of periclase was determined by burning magnesium metal in an oxygen-bomb calorimeter and assigning the enthalpy of formation calculated in that experiment to the mineral periclase. Magnesium oxide may be prepared in several ways, but one common procedure is to dehydrate brucite, $\text{Mg}(\text{OH})_2$. Taylor and Wells (1938) have shown that the procedure used to dehydrate a brucite sample affects the heat of solution of the resulting MgO sample. In dilute hydrochloric acid, the difference in the molar enthalpy of solution can be as large as 4 kJ. In this example, we can see that the enthalpy of formation of forsterite from the elements depends upon the procedure used to prepare the MgO sample. Because the thermodynamic properties of the MgO sample prepared by dehydration of brucite are not necessarily equivalent to those of the MgO sample produced in the oxygen-bomb experiment, the seemingly direct reference of forsterite to the element Mg is not simple and straightforward. The magnitude of the difference (the systematic error) between the thermodynamic properties of the MgO used as the secondary reference material in the dissolution reaction and the properties of the MgO formed in the oxygen-bomb calorimeter is the amount that the magnesium reference state is altered by the use of the dissolution reaction.

Helgeson and others (1978) have concluded that the generally accepted enthalpy and Gibbs free energies of formation of corundum (see, for example, CODATA, 1978) are in error by about 14 kJ. Hemingway and others (1978) and Hemingway and Robie (1977), on the other hand, have found the literature values for the enthalpy and Gibbs free energies of formation of corundum to be consistent with both calorimetric and phase-equilibrium data. Haas and others (1980, 1981) and, consequently, this study, and the data of Hemley and others (1980) support the conclusion of Hemingway and others (1978) regarding the consistency of the thermochemical data (relative stabilities) for the aluminum reference phases, gibbsite and corundum. Because the relative stabilities of all the aluminum-bearing phases appear to be well established from the calorimetric, silica-solubility, and phase-equilibrium data, it is obvious that the data of Helgeson and others (1978) listed in table 1 differ from the other three tabulations mainly in their reference value for aluminum.

The experimental results reported by Hemley and others (1980) were given to Helgeson and others (1978) and to Haas and others (1980, 1981) before publication. The results of Hemley and others were shown to be consistent within the analyzed data sets recommended by Helgeson and others and by Haas and others, although significantly different values were assigned to the enthalpies and free energies of for-

mation of the aluminum-bearing phases in those reports. Hemley and others referenced the aluminum-bearing phases to the thermochemical values for kaolinite given by Hemingway and others (1978) and Robie and others (1979), and, from their experimental data, they independently derived a value for the free energy of formation of corundum that was consistent with the value accepted by Haas and others, Robie and others, Hemingway and others, and in this study.

TABLE 1. — *Enthalpies of formation from the elements at 298.15 K for selected phases taken from several literature references*
[—, value not given]

Phase	Haas and others (1979)	Robie and others (1979)	Helgeson and others (1978)*	Hemley and others (1980)
Corundum Al_2O_3 -----	-1675.711	-1675.700	-1661.655	-1672.600
	± 1.000	± 1.300	(-1674.7)	± 6.0
Quartz SiO_2 -----	-910.699	-910.700	-910.648	-910.700
	± 900	± 1.000		± 1.00
Water H_2O -----	-285.808	-285.830	-285.830	-285.830
	± 0.42	± 0.42		± 0.4
Lime CaO -----	-635.094	-635.089	-635.089	-
	± 1.30	± 879		
Diaspore $AlO(OH)$ -----	-999.456	-1000.585	-992.319	-998.825
	± 366	± 5.000	(-998.8)	± 3.8
Boehmite $AlO(OH)$ -----	-990.424	-993.054	-983.566	-990.608
	± 725	± 2.110	(-989.1)	± 3.9
Gibbsite $Al(OH)_3$ -----	-1293.334	-1293.128	-1293.128	-
	± 628	± 1.192		
Kaolinite $Al_2Si_2O_5(OH)_4$ -----	-4119.780	-4120.114	-4109.613	-4120.114
	± 1.065	± 3.975	(-4122.6)	± 2.6
Pyrophyllite $Al_2Si_4O_{10}(OH)_2$ -----	-5642.023	-5639.800	-5628.790	-5640.415
	± 1.158	± 3.950	(-5641.8)	± 4.5
Kyanite Al_2SiO_5 -----	-2594.269	-2591.73 0	-2581.097	-2593.063
	± 433	± 1.900	(-2594.1)	± 5.8
Andalusite Al_2SiO_5 -----	-2590.270	-2587.525	-2576.783	-2588.663
	± 641	± 2.100	(-2589.8)	± 5.7
Sillimanite Al_2SiO_5 -----	-2587.774	-2585.760	-2573.574	-2585.341
	± 537	± 1.740	(-2586.6)	± 5.8
Anorthite $CaAl_2Si_2O_8$ -----	-4227.833	-4229.100	-4216.518	-
	± 1.118	± 3.125	(-4229.5)	
Gehlenite $Ca_2Al_2SiO_7$ -----	-3981.707	-4007.570	-3981.766	-
	± 2.458	± 2.820	(-3994.8)	
Grossular $Ca_3Al_2Si_3O_{12}$ -----	-6636.338	-6643.140	-6624.933	-
	± 3.220	± 6.000	(-6637.9)	
Ca-Al pyroxene $CaAl_2SiO_6$ -----	-3298.956	-3275.680	-3280.310	-
	± 1.912	± 2.761	(-3293.3)	
Margarite $CaAl_2Si_2O_{10}(OH)_2$ -----	-6240.601	-	-6217.520	-
	± 1.954		(-6243.5)	
Prehnite $Ca_2Al_2Si_3O_{10}(OH)_2$ -----	-6193.631	-	-6201.060	-
	± 1.699		(-6214.1)	
Zoisite $Ca_2Al_2Si_3O_{12}(OH)$ -----	-6891.147	-	-6879.044	-
	± 2.080		(-6892.0)	
Wollastonite $CaSiO_3$ -----	-1634.766	-1635.200	-1630.965	-
	± 702	± 1.435		

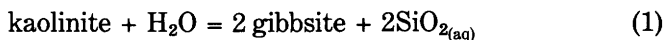
*The values in parentheses represent the value derived by Helgeson and others plus a correction of -6.5 kJ per mole of aluminum.

We shall discuss the differences in the tabulated thermodynamic data in terms of the reported differences in the enthalpy of formation, rather than in terms of differences in the Gibbs free energy of formation, because (1) all the tabulations use essentially the same values for the entropy of the condensed phases, (2) the standard reference

pressure used by Haas and others and Helgeson and others differs from that used by Robie and others and in this study, and (3) the enthalpy of formation is relatively insensitive to small pressure changes.

The difference between the enthalpies of formation given by Helgeson and others (1978) for the aluminum-bearing phases listed in table 1 and the enthalpies of formation for the same phases taken from the other sources listed averages roughly -6.5 kJ for each mole of aluminum (range about -5 to -7 kJ). This difference was added to the value for the enthalpy of formation of each aluminum-bearing phase taken from Helgeson and others, and the corrected results are listed in table 1 immediately below the original values. The only exception was the enthalpy of formation of gibbsite, which had been taken directly from Hemingway and Robie (1977) and had not been a variable parameter in the analysis by Helgeson and others. A comparison of the adjusted data set with the other thermochemical data in table 1 shows the data from all tabulations to be in good agreement, with a few exceptions (for example, gehlenite).

An examination of the data and procedures used by Helgeson and others (1978) and by Robie and others (1979), Hemley and others (1980), and Haas and others (1979, 1980, 1981) reveals that the difference in the aluminum reference state arises from the use of different experimental data to obtain the enthalpy of formation of kaolinite. Helgeson and others calculated the enthalpy of formation of kaolinite by using reaction 1 and the thermodynamic data for gibbsite, water, and aqueous silica as given in Hemingway and Robie (1977), Robie and others (1979), and Walther and Helgeson (1977), respectively, and from the composition of mineral assemblages and presumably coexisting natural waters in Jamaican bauxite deposits and in weathered basalts from Hawaii taken from Hill and Ellington (1961), Patterson and Roberson (1961), Garrels and Mackenzie (1967), and Bricker and Garrels (1967).



Patterson and Roberson (1961) discussed the mineralogy of the sites where they collected the water samples referenced by Helgeson and others (1978). The Hawaiian soils contained high concentrations of gibbsite associated with small amounts of clay near the surface. The clay gradually increased to more than 50 percent of the soil volume at greater depths where gibbsite became a minor constituent. Patterson and Roberson noted that all the clay belonged to the kaolin group, halloysite being the most common or possibly the only member present. Hill and Ellington (1961) described the Jamaican soil as ranging from a transported bauxitic laterite to a mixture of kaolinite and montmorillonite. Hem and others (1973) concluded that reaction 1 should be

viewed as an equilibrium between the silica dissolved in the ground water and halloysite and (or) microcrystalline gibbsite.

We are aware of only two experimental studies (Kittrick, 1967, 1980) that bear directly upon the interpretation of reaction 1. Kittrick (1967) determined the solubility of gibbsite and kaolinite (labeled Georgia 3) separately and in combination. Kittrick observed that the calculated free energy of formation of kaolinite determined from a solution equilibrated with both kaolinite and gibbsite was consistent with a value calculated from the dissolution of kaolinite alone. The free energy of formation of gibbsite calculated from the kaolinite-gibbsite solution was in good agreement with the results obtained in an earlier set of experiments (Kittrick, 1966a) on the same gibbsite sample.

Interpretation of the results presented by Kittrick (1967) is not straightforward. Kittrick (1966b) showed that the free energy of formation calculated for the Georgia 3 kaolinite sample varied. Removal of particles smaller than 2μ resulted in a change of 2.5 kJ/mol in the calculated free energy of the sample. Kittrick (1966b) attributed the difference in the equilibrium solubility for the Georgia 3 kaolinite and that part of the sample having grain size larger than 2μ to the presence of amorphous material in the $<2\mu$ -sized fraction that controlled the solubility. In addition, the free energy of formation of the coarse fraction of the Georgia 3 kaolinite was 2.1 kJ/mol more positive than the free energy of formation that Kittrick (1966b) felt best represented crystalline kaolinite. To further complicate the problem, Kittrick (1967) used the coarse fraction of the Georgia 3 kaolinite sample, but the calculated free energy he obtained for kaolinite from the mixed kaolinite-gibbsite sample was consistent with his earlier result (Kittrick, 1966b) for the $<2\mu$ -sized fraction.

Taking Kittrick's (1967) results at face value, we recalculated the free energy of formation of the Georgia 3 kaolinite sample using the necessary ancillary data of Robie and others (1979) and obtained -3787.8 kJ/mol for the "kaolinite" phase in equilibrium with macrocrystalline gibbsite. This value is in excellent agreement with the free energy of formation calculated by Helgeson and others (1978), although Helgeson and others do not specifically reference Kittrick (1967) in their discussion of kaolinite. Furthermore, the result is in excellent agreement with the free energy of formation derived from the study in which the solubility was controlled by the amorphous portion of the Georgia 3 kaolinite phase (Kittrick, 1966b) and is 6 kJ/mol of kaolinite more positive than the free energy of formation of well-crystallized kaolinite given by Kittrick (1966b) as recalculated by Hemingway and others (1978). Kittrick (1980) obtained results similar to those of his earlier studies through the immiscible-displacement method.

The results presented by Kittrick (1966a, b; 1967; 1970; 1980) clearly show a wide range of silica concentrations in "equilibrium" with a fixed alumina concentration in aqueous solutions equilibrated with mixed samples of gibbsite and kaolinite at 298.15 K. Hence, it is doubtful that an average silica value taken from natural water analyses (the procedure followed by Helgeson and others, 1978, in using reaction 1) would represent well-crystallized kaolinite, a point also made by Paces (1978). Hemley and others (1980) suggested that use of the least soluble data point on the plot of compositions of waters from bauxite soils would yield a result consistent with their results and with those of Hemingway and others (1978). The evidence presented in this study strongly suggests that the use of reaction 1 by Helgeson and others (1978) to establish the thermochemical data for kaolinite was incorrect. Consequently, the aluminum reference state appears to have been redefined by Helgeson and others through their use of reaction 1; that is, kaolinite as defined by Helgeson and others became the secondary aluminum reference standard in their data set.

CONFIDENCE LIMITS

The 2-sigma confidence limits assigned at 298.15 K reflect only the variation in the final set of data in the chemical system. They do not include confidence limits on the reference data or confidence limits assigned to the original experimental data, as was done by Robie and others (1979). For this reason, the confidence limits for formation from the elements and from the oxides are identical.

The data were weighted by the reciprocal of the precision, which allowed the simultaneous fitting of properties whose values vary over several orders of magnitude; this procedure constrained the solutions toward the more precise observations. Error plots of the weighted difference, (observed - calculated)/reported precision, plotted as a function of temperature allowed rapid identification of discordant data. The errors should not exceed the ± 2 sigma assigned to the experimental observation. A complete discussion of this point is given in Haas and Fisher (1976) and in Haas and others (1981).

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PROPERTIES AT HIGH TEMPERATURES

15

Corundum

FORMULA WEIGHT 101.961

Al₂O₃: (Corundum), crystals 298.15 to melting point 2345 K.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(C _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	50.92	50.92	79.39	-1675.711	-1582.242	277.203
UNCERTAINTY		0.20	0.20	0.04	1.000	1.100	0.193
400	22.455	76.72	54.26	95.58	-1676.363	-1550.168	202.432
500	38.144	99.19	61.05	105.53	-1676.109	-1518.639	158.652
600	49.968	119.06	69.09	112.25	-1675.406	-1487.208	129.474
700	59.226	136.74	77.52	117.03	-1674.521	-1455.914	108.642
800	66.682	152.61	85.93	120.54	-1673.635	-1424.737	93.026
900	72.821	166.97	94.15	123.22	-1672.887	-1393.673	80.887
1000	77.970	180.07	102.10	125.31	-1693.674	-1361.150	71.099
1100	82.353	192.09	109.74	127.00	-1692.665	-1327.940	63.059
1200	86.134	203.20	117.07	128.42	-1691.569	-1294.838	56.363
1300	89.435	213.53	124.10	129.65	-1690.394	-1261.801	50.700
1400	92.349	223.18	130.83	130.77	-1689.156	-1228.897	45.851
1500	94.946	232.24	137.30	131.83	-1687.850	-1196.062	41.651
1600	97.283	240.78	143.50	132.86	-1686.483	-1163.327	37.979
1700	99.406	248.87	149.46	133.90	-1685.045	-1130.699	34.742
1800	101.352	256.55	155.20	134.97	-1683.537	-1098.110	31.866

MELTING POINT	2345	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	10.016	kJ	MOLAR VOLUME	2.5575 J/bar 25.575 cm ³

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 233.004 - 1.95913 \times 10^{-2} T + 9.44410 \times 10^{-6} T^2 - 2.46518 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

16 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

AlO(OH) - Reference

FORMULA WEIGHT 59.988

AlO(OH): Diaspore crystals 298.15 to 571.86 K. Boehmite 571.86 to 800 K.

TEMP. K	$(H_T^\circ - H_{298}^\circ)/T$ J/mol·K	S_T° J/mol·K	$-(G_T^\circ - H_{298}^\circ)/T$ J/mol·K	C_P° J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	35.34	35.34	53.10	-999.456	-920.896	161.338
UNCERTAINTY		0.09	0.09	0.09	(0.366)	(0.362)	(0.063)
400	15.212	52.81	37.60	65.57	-1000.425	-893.875	116.729
500	26.190	68.41	42.22	74.16	-1000.561	-867.210	90.597
571.86	32.527	78.70	46.17	78.95	-1000.281	-848.058	77.463
571.86	56.738	102.90	46.17	100.86	-986.436	-848.058	77.463
600	58.855	107.81	48.95	103.21	-985.701	-841.270	73.239
700	65.730	124.28	58.55	110.49	-982.580	-817.442	60.999
800	71.710	139.44	67.73	116.45	-979.033	-794.084	51.849

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^\circ - H_0^\circ$	kJ	MOLAR VOLUME	1.7760 J/bar 17.760 cm ³
TRANSITIONS IN REFERENCE STATE ELEMENTS			
ALUMINUM... M. P. 933 K.			

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 150.556 - 1.73002 \times 10^3 T^{-0.5} + 2.43069 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 200 - 800 K, diaspore)

$$C_P^\circ = 206.903 - 2.59274 \times 10^3 T^{-0.5} + 7.77112 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 200 - 800 K, boehmite)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

17

Diaspore

FORMULA WEIGHT 59.988

AlO(OH): Crystals 298.15 to 800 K. See reference table for AlO(OH).

TEMP. K	$(H_T^\circ - H_{298}^\circ)/T$ J/mol·K	S_T° J/mol·K	$-(C_T^\circ - H_{298}^\circ)/T$ J/mol·K	C_P° J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	35.34	35.34	53.10	-999.456	-920.896	161.338
UNCERTAINTY		0.09	0.09	0.09	(0.366)	(0.362)	(0.063)
400	15.212	52.81	37.60	65.57	-1000.425	-893.875	116.729
500	26.190	68.41	42.22	74.16	-1000.561	-867.210	90.597
600	34.745	82.53	47.78	80.60	-1000.167	-840.569	73.178
700	41.670	95.35	53.68	85.66	-999.422	-814.029	60.744
800	47.435	107.06	59.63	89.77	-998.453	-787.604	51.426

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^\circ - H_0^\circ$	kJ	MOLAR VOLUME	1.7760 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS			17.760 cm ³
ALUMINUM... M. P. 933 K.			

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 150.556 - 1.73002 \times 10^3 T^{-0.5} + 2.43069 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 200 - 800 K)

COMPILED 9-30-79

18 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Boehmite FORMULA WEIGHT 59.988

AlO(OH): Crystals 298.15 to 800 K. See reference table for AlO(OH).

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^\circ - H_{298}^\circ)/T$ J/mol·K	S_T° J/mol·K	$-(G_T^\circ - H_{298}^\circ)/T$ J/mol·K	C_P° J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	48.43	48.43	65.49	-990.424	-915.768	160.439
UNCERTAINTY		0.51	0.51	0.22	(0.725)	(0.682)	(0.119)
400	18.912	70.14	51.23	82.12	-989.913	-890.297	116.261
500	32.806	89.81	57.01	94.06	-988.221	-865.570	90.426
600	43.808	107.81	64.00	103.21	-985.697	-841.266	73.239
700	52.833	124.28	71.45	110.49	-982.576	-817.438	60.998
800	60.425	139.44	79.01	116.45	-979.029	-794.080	51.848

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

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 206.903 - 2.59274 \times 10^3 T^{-0.5} + 7.77112 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 200 - 800 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

19

Gibbsite FORMULA WEIGHT 78.003

Al(OH)₃: Crystals 298.15 to 800 K. Gibbsite decomposes above 480 K at 1 bar.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^\circ - H_{298}^\circ)/T$ J/mol·K	S_T° J/mol·K	$-(G_T^\circ - H_{298}^\circ)/T$ J/mol·K	C_p° J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	68.44	68.44	91.73	-1293.334	-1155.099	202.369
UNCERTAINTY		0.34	0.34	0.16	(0.628)	(0.637)	(0.112)
400	26.537	98.90	72.36	115.66	-1294.248	-1107.667	144.647
500	46.284	126.77	80.49	134.26	-1293.323	-1061.102	110.853
600	62.280	152.67	90.39	149.86	-1290.964	-1014.854	88.351
700	75.783	176.81	101.03	163.47	-1287.422	-969.108	72.316
800	87.519	199.45	111.93	175.67	-1282.883	-923.930	60.327

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^\circ - H_0^\circ$	12.719 kJ	MOLAR VOLUME	3.1956 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS			31.956 cm ³

ALUMINUM... M. P. 933 K.

HEAT CAPACITY EQUATION(S)

$$C_p^\circ = 220.851 + 3.00646 \times 10^{-2} T - 2.66764 \times 10^{-3} T^{-0.5} + 6.61704 \times 10^{-5} T^{-2}$$

(EQUATION VALID FROM 200 - 800 K)

COMPILED 9-30-79

20 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Line FORMULA WEIGHT 56.079

CaO: Crystals 298.15 to 1800K.

TEMP. K	$(H_T^\circ - H_{298}^\circ)/T$ J/mol·K	S_T° J/mol·K	$-(G_T^\circ - H_{298}^\circ)/T$ J/mol·K	C_P° J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY	FREE ENERGY	LOG K
					kJ/mol	kJ/mol	
298.15	0.000	38.10	38.10	42.15	-635.094	-603.464	105.725
UNCERTAINTY		0.10	0.10	0.08	1.300	1.320	0.231
400	11.325	51.14	39.82	46.38	-634.697	-592.704	77.399
500	18.600	61.77	43.17	48.82	-634.152	-582.268	60.829
600	23.780	70.83	47.05	50.45	-633.624	-571.939	49.792
700	27.677	78.70	51.02	51.62	-633.212	-561.698	41.915
800	30.727	85.65	54.92	52.51	-633.712	-551.412	36.004
900	33.190	91.88	58.69	53.23	-633.594	-541.126	31.406
1000	35.225	97.52	62.29	53.84	-633.852	-530.841	27.728
1100	36.943	102.68	65.73	54.38	-634.490	-520.515	24.717
1200	38.416	107.43	69.01	54.86	-642.459	-509.491	22.178
1300	39.698	111.84	72.14	55.32	-641.672	-498.449	20.028
1400	40.831	115.95	75.12	55.77	-640.857	-487.465	18.188
1500	41.841	119.82	77.97	56.21	-640.011	-476.534	16.594
1600	42.752	123.46	80.71	56.65	-639.136	-465.669	15.203
1700	43.584	126.91	83.32	57.11	-638.227	-454.851	13.976
1800	44.348	130.18	85.84	57.58	-790.783	-440.728	12.790

MELTING POINT	3200	K	BOILING POINT	K
ENTHALPY OF MELTING	79.496	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^\circ - H_0^\circ$	6.749	kJ	MOLAR VOLUME	1.6764 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS				16.764 cm ³

CALCIUM.... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 71.6851 - 3.08248 \times 10^{-3} T + 2.23862 \times 10^{-6} T^2 - 4.31990 \times 10^{-2} T^{-0.5} - 2.55577 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

21

H₂O reference FORMULA WEIGHT 18.015

H₂O: Liquid 298.15 to 372.8 K. Ideal gas 372.8 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS							
	(H _T ^o -H ₂₉₈ ^o)/T		S _T ^o	-(C _T ^o -H ₂₉₈ ^o)/T	C _P ^o	ENTHALPY	GIBBS FREE ENERGY	LOG K
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	69.92	69.92	75.25	-285.808	-237.111	41.541	
UNCERTAINTY		0.08	0.08	0.15	0.042	0.084	0.015	
372.8	15.094	86.76	71.67	75.99	-283.461	-225.099	31.540	
372.8	124.724	196.40	71.68	34.04	-242.591	-225.103	31.541	
400	118.563	198.80	80.24	34.24	-242.858	-223.913	29.240	
500	101.786	206.53	104.75	35.15	-243.846	-219.063	22.885	
600	90.772	213.04	122.27	36.25	-244.785	-214.014	18.632	
700	83.067	218.72	135.65	37.46	-245.662	-208.820	15.582	
800	77.445	223.80	146.36	38.71	-246.471	-203.500	13.287	
900	73.212	228.43	155.22	39.99	-247.211	-198.076	11.496	
1000	69.953	232.71	162.76	41.25	-247.883	-192.587	10.060	
1100	67.401	236.70	169.30	42.49	-248.487	-187.024	8.881	
1200	65.376	240.45	175.08	43.69	-249.030	-181.408	7.897	
1300	63.752	244.00	180.24	44.85	-249.514	-175.760	7.062	
1400	62.441	247.36	184.92	45.94	-249.945	-170.077	6.346	
1500	61.377	250.57	189.19	46.98	-250.325	-164.353	5.723	
1600	60.508	253.63	193.12	47.95	-250.661	-158.606	5.178	
1700	59.796	256.56	196.77	48.86	-250.958	-152.850	4.697	
1800	59.212	259.38	200.17	49.69	-251.222	-147.076	4.268	

MELTING POINT	273.15 K	BOILING POINT	372.8 K
ENTHALPY OF MELTING	6.008 kJ	ENTHALPY OF VAPORIZATION	40.870 kJ
H ₂₉₈ ^o - H ₀ ^o	13.293 kJ	MOLAR VOLUME	1.8069 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS			18.069 cm ³

HEAT CAPACITY EQUATION(S)

$$C_P^o = 42.0228 + 3.49132 \times 10^2 T + 1.10338 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 273 - 425 K, liquid)

$$C_P^o = 10.4381 + 1.29775 \times 10^{-2} T - 4.46885 \times 10^{-6} T^2 + 2.99188 \times 10^2 T^{-0.5}$$

$$- 1.31077 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 298 - 1800 K, gas)

COMPILED 9-30-79

22 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Quartz FORMULA WEIGHT 60.085

SiO₂: Alpha quartz 298.15 to 844 K. Beta quartz 844 to 1800 K.

Beta quartz is metastable above 1140 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^\circ - H_{298}^\circ)/T$	S_T°	$-(G_T^\circ - H_{298}^\circ)/T$	C_P°	ENTHALPY	FREE ENERGY	LOG 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	44.75	-910.699	-856.288	150.019
UNCERTAINTY		0.40	0.40	0.04	0.900	0.900	0.158
<hr/>							
400	12.520	55.85	43.33	53.14	-910.869	-837.657	109.387
500	21.298	68.41	47.11	59.44	-910.578	-819.383	85.601
600	28.102	79.72	51.62	64.67	-909.926	-801.195	69.751
700	33.657	90.04	56.38	69.22	-908.958	-783.147	58.439
800	38.364	99.55	61.19	73.32	-907.699	-765.255	49.966
844	40.230	103.53	63.29	75.01	-907.015	-757.364	46.873
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844	41.135	104.43	63.29	67.39	-906.251	-757.364	46.873
900	42.786	108.78	65.99	67.95	-905.872	-747.569	43.388
1000	45.352	115.99	70.64	68.95	-905.116	-730.024	38.133
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1100	47.543	122.61	75.06	69.96	-904.347	-712.558	33.837
1200	49.452	128.74	79.28	70.96	-903.552	-695.145	30.259
1300	51.146	134.46	83.31	71.96	-902.723	-677.819	27.235
1400	52.669	139.83	87.16	72.97	-901.854	-660.560	24.646
1500	54.055	144.90	90.84	73.97	-900.937	-643.349	22.403
1600	55.332	149.70	94.37	74.98	-899.967	-626.210	20.444
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1700	56.517	154.28	97.76	75.98	-949.449	-608.696	18.703
1800	57.626	158.65	101.02	76.98	-948.075	-588.684	17.083

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ [°] - H ₀ [°]	6.916 kJ	MOLAR VOLUME	2.2688 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS			22.688 cm ³

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 83.2101 + 1.09962 \times 10^{-2} T - 7.77338 \times 10^{-2} T^{-0.5}$$

(EQUATION VALID FROM 200 - 844 K)

$$C_P^\circ = 58.9107 + 5.02080 \times 10^{-3} T$$

(EQUATION VALID FROM 844 - 1800 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

23

Al₂SiO₅ - Reference

FORMULA WEIGHT 162.046

Al₂SiO₅: Kyanite crystals 298.15 to 430.46 K. Andalusite crystals 430.46 to 1016.9 K. Sillimanite crystals 1016.9 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GTBBS						
	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	84.47	84.47	122.35	-2594.269	-2444.032	428.186
UNCERTAINTY		0.44	0.44	0.15	(0.433)	(0.389)	(0.068)
400	34.662	124.29	89.62	147.86	-2595.216	-2392.497	312.429
430.46	42.875	135.35	92.47	153.47	-2594.847	-2377.403	288.490
430.46	52.084	144.56	92.47	153.27	-2590.883	-2377.403	288.490
500	66.904	168.29	101.39	163.49	-2590.815	-2342.497	244.720
600	83.910	199.07	115.16	173.66	-2589.687	-2292.927	199.618
700	97.246	226.38	129.13	180.42	-2588.284	-2243.582	167.419
800	107.954	250.79	142.84	185.14	-2586.867	-2194.427	143.282
900	116.736	272.81	156.08	188.71	-2585.602	-2145.444	124.519
1000	124.086	292.86	168.77	191.73	-2605.885	-2095.071	109.436
1016.90	125.214	296.07	170.86	192.21	-2605.528	-2085.805	107.141
1016.90	128.133	298.99	170.86	194.96	-2602.560	-2085.805	107.141
1100	133.269	314.40	181.13	197.21	-2601.160	-2044.313	97.077
1200	138.692	331.65	192.96	199.38	-2599.254	-1993.769	86.787
1300	143.428	347.68	204.25	201.07	-2597.276	-1943.378	78.086
1400	147.594	362.63	215.04	202.37	-2595.262	-1893.180	70.636
1500	151.279	376.63	225.35	203.34	-2593.229	-1843.089	64.182
1600	154.556	389.78	235.22	204.04	-2591.203	-1793.153	58.541
1700	157.482	402.16	244.68	204.51	-2639.703	-1742.929	53.554
1800	160.103	413.86	253.76	204.78	-2637.446	-1690.213	49.049

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	16.041 kJ	MOLAR VOLUME	4.4090 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS			44.090 cm ³

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 336.114 - 1.29800 \times 10^{-2} T + 3.55746 \times 10^{-5} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1600 K, kyanite)

$$C_P^o = 543.227 - 0.103545 T + 6.68935 \times 10^{-5} T^2 - 6.75436 \times 10^{-3} T^{-0.5}$$

$$+ 2.28751 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K, andalusite)

$$C_P^o = 313.470 - 9.47081 \times 10^{-3} T + 3.16487 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1800 K, sillimanite)

COMPILED 9-30-79

24 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Al₂SiO₅ - Reference FORMULA WEIGHT 162.046

Al₂SiO₅: Kyanite crystals 298.15 to 430.46 K. Andalusite crystals 430.46 to 1016.9 K. Sillimanite crystals 1016.9 to 1800 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS						
	(H _T ^o -H ₂₉₈ ^o)/T	S _T ^o	-(G _T ^o -H ₂₉₈ ^o)/T	C _P ^o	ENTHALPY	FREE ENERGY	LOG K
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	84.47	84.47	122.35	-7.859 *	-5.502 *	0.964
UNCERTAINTY		0.44	0.44	0.15	0.433	0.389	0.068
400	34.662	124.29	89.62	147.86	-7.984 *	-4.673 *	0.610
430.46	42.875	135.35	92.47	153.47	-8.009 *	-4.420 *	0.536
430.46	52.084	144.56	92.47	153.27	-4.045 *	-4.420 *	0.536
500	66.904	168.29	101.39	163.49	-4.128 *	-4.474 *	0.467
600	83.910	199.07	115.16	173.66	-4.355 *	-4.524 *	0.394
700	97.246	226.38	129.13	180.42	-4.805 *	-4.521 *	0.337
800	107.954	250.79	142.84	185.14	-5.533 *	-4.434 *	0.290
900	116.736	272.81	156.08	188.71	-6.843 *	-4.202 *	0.244
1000	124.086	292.86	168.77	191.73	-7.095 *	-3.897 *	0.204
1016.90	125.214	296.07	170.86	192.21	-7.138 *	-3.842 *	0.197
1016.90	128.133	298.99	170.86	194.96	-4.170 *	-3.842 *	0.197
1100	133.269	314.40	181.13	197.21	-4.148 *	-3.815 *	0.181
1200	138.692	331.65	192.96	199.38	-4.133 *	-3.785 *	0.165
1300	143.428	347.68	204.25	201.07	-4.159 *	-3.757 *	0.151
1400	147.594	362.63	215.04	202.37	-4.252 *	-3.724 *	0.139
1500	151.279	376.63	225.35	203.34	-4.442 *	-3.669 *	0.128
1600	154.556	389.78	235.22	204.04	-4.753 *	-3.617 *	0.118
1700	157.482	402.16	244.68	204.51	-5.209 *	-3.534 *	0.109
1800	160.103	413.86	253.76	204.78	-5.834 *	-3.418 *	0.099

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	16.041 kJ	MOLAR VOLUME	4.4090 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES			44.090 cm ³

SiO₂..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 336.114 - 1.29800 \times 10^{-2} T + 3.55746 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1600 K, kyanite)

$$C_P^o = 543.227 - 0.103545 T + 6.68935 \times 10^{-5} T^2 - 6.75436 \times 10^{-3} T^{-0.5}$$

$$+ 2.28751 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K, andalusite)

$$C_P^o = 313.470 - 9.47081 \times 10^{-3} T + 3.16487 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1800 K, sillimanite)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

25

Kyanite

FORMULA WEIGHT 162.046

Al₂SiO₅: Crystals 298.15 to 1600 K. See Al₂SiO₅ reference table.

TEMP.	FORMATION FROM THE ELEMENTS						
	$(H_T^\circ - H_{298}^\circ)/T$	S_T°	$-(C_T^\circ - H_{298}^\circ)/T$	C_P°	ENTHALPY	GIBBS FREE ENERGY	LOG K
K	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	84.47	84.47	122.35	-2594.269	-2444.032	428.186
UNCERTAINTY		0.44	0.44	0.15	(0.433)	(0.389)	(0.068)
400	34.662	124.29	89.62	147.86	-2595.216	-2392.497	312.429
500	59.024	159.14	100.11	164.04	-2594.755	-2341.858	244.653
600	77.518	190.10	112.58	175.31	-2593.522	-2291.381	199.483
700	92.101	217.77	125.67	183.48	-2591.885	-2241.155	167.238
800	103.924	242.68	138.76	189.57	-2590.091	-2191.163	143.069
900	113.707	265.29	151.58	194.17	-2588.328	-2141.398	124.284
1000	121.935	285.94	164.00	197.66	-2608.036	-2090.303	109.187
1100	128.945	304.91	175.96	200.30	-2605.917	-2038.631	96.807
1200	134.977	322.42	187.45	202.27	-2603.712	-1987.150	86.499
1300	140.212	338.67	198.46	203.70	-2601.457	-1935.847	77.784
1400	144.784	353.81	209.02	204.69	-2599.195	-1884.758	70.321
1500	148.801	367.95	219.15	205.32	-2596.947	-1833.793	63.859
1600	152.345	381.22	228.87	205.64	-2594.741	-1782.995	58.209

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ [°] - H ₀ [°]	16.041 kJ	MOLAR VOLUME	4.4090 J/bar 44.090 cm ³

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 336.114 - 1.29800 \times 10^{-2} T - 3.55746 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1600 K)

COMPILED 9-30-79

26 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Kyanite

FORMULA WEIGHT 162.046

Al₂SiO₅: Crystals 298.15 to 1600 K. See Al₂SiO₅ reference table.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	84.47	84.47	122.35	-7.859 *	-5.502 *	0.964
UNCERTAINTY		0.44	0.44	0.15	0.433	0.389	0.068
400	34.662	124.29	89.62	147.86	-7.984 *	-4.673 *	0.610
500	59.024	159.14	100.11	164.04	-8.068 *	-3.835 *	0.401
600	77.518	190.10	112.58	175.31	-8.190 *	-2.978 *	0.259
700	92.101	217.77	125.67	183.48	-8.406 *	-2.094 *	0.156
800	103.924	242.68	138.76	189.57	-8.757 *	-1.170 *	0.076
900	113.707	265.29	151.58	194.17	-9.569 *	-0.156 *	0.009
1000	121.935	285.94	164.00	197.66	-9.246 *	0.871 *	-0.046
1100	128.945	304.91	175.96	200.30	-8.905 *	1.867 *	-0.089
1200	134.977	322.42	187.45	202.27	-8.591 *	2.834 *	-0.123
1300	140.212	338.67	198.46	203.70	-8.340 *	3.774 *	-0.152
1400	144.784	353.81	209.02	204.69	-8.185 *	4.698 *	-0.175
1500	148.801	367.95	219.15	205.32	-8.160 *	5.627 *	-0.196
1600	152.345	381.22	228.87	205.64	-8.291 *	6.541 *	-0.214

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	16.041 kJ	MOLAR VOLUME	4.4090 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES			44.090 cm ³
SiO ₂ ALPHA - BETA TRANSITION 844 K.			

HEAT CAPACITY EQUATION(S)

$$C_P^o = 336.114 - 1.29800 \times 10^{-2} T + 3.55746 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1600 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

27

Andalusite

FORMULA WEIGHT 162.046

Al₂SiO₅: Crystals 298.15 to 1800 K. See Al₂SiO₅ reference table.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS				ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(C _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K			
298.15	0.000	93.77	93.77	121.99	-2590.270	-2442.808	427.972
UNCERTAINTY		0.73	0.73	0.26	(0.641)	(0.484)	(0.085)
400	34.587	133.51	98.92	147.67	-2591.247	-2392.217	312.393
500	58.906	168.29	109.39	163.49	-2590.815	-2342.497	244.720
600	77.245	199.07	121.82	173.66	-2589.687	-2292.928	199.618
700	91.533	226.38	134.85	180.42	-2588.284	-2243.582	167.419
800	102.954	250.80	147.84	185.14	-2586.868	-2194.429	143.282
900	112.291	272.81	160.52	188.71	-2585.603	-2145.446	124.519
1000	120.087	292.86	172.77	191.73	-2605.885	-2095.071	109.436
1100	126.730	311.26	184.53	194.61	-2604.354	-2044.063	97.065
1200	132.512	328.33	195.81	197.65	-2602.671	-1993.194	86.762
1300	137.651	344.28	206.63	201.08	-2600.787	-1942.466	78.050
1400	142.320	359.32	217.00	205.06	-2598.646	-1891.930	70.589
1500	146.654	373.62	226.97	209.72	-2596.168	-1841.524	64.128
1600	150.762	387.33	236.57	215.16	-2593.275	-1791.312	58.481
1700	154.731	400.56	245.83	221.47	-2640.381	-1740.882	53.491
1800	158.635	413.42	254.78	228.70	-2636.090	-1688.061	48.986

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	17.096 kJ	MOLAR VOLUME	5.1530 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS			51.530 cm ³

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 543.227 - 0.103545 T + 6.68935 \times 10^{-5} T^2 - 6.75436 \times 10^{-3} T^{-0.5} + 2.28751 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

28 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Andalusite

FORMULA WEIGHT 162.046

Al_2SiO_5 : Crystals 298.15 to 1800 K. See Al_2SiO_5 reference table.

TEMP. K	FORMATION FROM THE OXIDES GIBBS						
	$(H_T^\circ - H_{298}^\circ)/T$	S_T°	$-(G_T^\circ - H_{298}^\circ)/T$	C_P°	ENTHALPY	FREE ENERGY	LOG K
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	93.77	93.77	121.99	-3.860 *	-4.278 *	0.749
UNCERTAINTY		0.73	0.73	0.26	0.641	0.484	0.085
400	34.587	133.51	98.92	147.67	-4.015 *	-4.393 *	0.574
500	58.906	168.29	109.39	163.49	-4.128 *	-4.474 *	0.467
600	77.245	199.07	121.82	173.66	-4.355 *	-4.525 *	0.394
700	91.533	226.38	134.85	180.42	-4.805 *	-4.521 *	0.337
800	102.954	250.80	147.84	185.14	-5.534 *	-4.436 *	0.290
900	112.291	272.81	160.52	188.71	-6.844 *	-4.204 *	0.244
1000	120.087	292.86	172.77	191.73	-7.095 *	-3.897 *	0.204
1100	126.730	311.26	184.53	194.61	-7.342 *	-3.565 *	0.169
1200	132.512	328.33	195.81	197.65	-7.550 *	-3.210 *	0.140
1300	137.651	344.28	206.63	201.08	-7.670 *	-2.845 *	0.114
1400	142.320	359.32	217.00	205.06	-7.636 *	-2.474 *	0.092
1500	146.654	373.62	226.97	209.72	-7.381 *	-2.103 *	0.073
1600	150.762	387.33	236.57	215.16	-6.825 *	-1.775 *	0.058
1700	154.731	400.56	245.83	221.47	-5.887 *	-1.486 *	0.046
1800	158.635	413.42	254.78	228.70	-4.478 *	-1.266 *	0.037

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^\circ - H_0^\circ$	17.096 kJ	MOLAR VOLUME	5.1530 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES			51.530 cm ³
SiO ₂ ALPHA - BETA TRANSITION 844 K.			

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 543.227 - 0.103545 T + 6.68935 \times 10^{-5} T^2 - 6.75436 \times 10^{-3} T^{-0.5} + 2.28751 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

29

Sillimanite

FORMULA WEIGHT 162.046

Al₂SiO₅: Crystals 298.15 to 1800 K. See Al₂SiO₅ reference table.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H _T ^o -H ₂₉₈ ^o)/T	S _T ^o	-(C _T ^o -H ₂₉₈ ^o)/T	C _P ^o	ENTHALPY	FREE ENERGY	LOG K
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	96.09	96.09	124.53	-2587.774	-2441.002	427.655
UNCERTAINTY		0.55	0.55	0.16	(0.537)	(0.443)	(0.078)
400	34.885	136.19	101.30	147.65	-2588.632	-2390.673	312.191
500	59.014	170.83	111.82	162.46	-2588.265	-2341.214	244.586
600	77.172	201.42	124.25	172.90	-2587.235	-2291.890	199.528
700	91.423	228.68	137.26	180.59	-2585.865	-2242.776	167.359
800	102.949	253.19	150.25	186.42	-2584.376	-2193.857	143.245
900	112.484	275.42	162.94	190.93	-2582.933	-2145.123	124.500
1000	120.512	295.73	175.22	194.45	-2602.964	-2095.023	109.433
1100	127.365	314.40	187.03	197.21	-2601.160	-2044.314	97.077
1200	133.279	331.65	198.37	199.38	-2599.254	-1993.769	86.787
1300	138.431	347.68	209.25	201.07	-2597.277	-1943.380	78.086
1400	142.954	362.63	219.68	202.37	-2595.263	-1893.181	70.636
1500	146.949	376.63	229.68	203.34	-2593.230	-1843.092	64.182
1600	150.496	389.78	239.28	204.04	-2591.204	-1793.156	58.541
1700	153.661	402.16	248.50	204.51	-2639.704	-1742.930	53.554
1800	156.494	413.86	257.36	204.78	-2637.447	-1690.214	49.049

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	17.414 kJ	MOLAR VOLUME	4.9900 J/bar 49.900 cm ³

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

SILICON... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 313.470 - 9.47081 \times 10^{-3} T + 3.16487 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

Sillimanite

FORMULA WEIGHT 162.046

Al₂SiO₅: Crystals 298.15 to 1800 K. See Al₂SiO₅ reference table.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	96.09	96.09	124.53	-1.364 *	-2.472 *	0.433
UNCERTAINTY		0.55	0.55	0.16	0.537	0.443	0.078
400	34.885	136.19	101.30	147.65	-1.400 *	-2.849 *	0.372
500	59.014	170.83	111.82	162.46	-1.578 *	-3.192 *	0.333
600	77.172	201.42	124.25	172.90	-1.903 *	-3.487 *	0.304
700	91.423	228.68	137.26	180.59	-2.386 *	-3.715 *	0.277
800	102.949	253.19	150.25	186.42	-3.042 *	-3.864 *	0.252
900	112.484	275.42	162.94	190.93	-4.174 *	-3.881 *	0.225
1000	120.512	295.73	175.22	194.45	-4.174 *	-3.849 *	0.201
1100	127.365	314.40	187.03	197.21	-4.148 *	-3.816 *	0.181
1200	133.279	331.65	198.37	199.38	-4.133 *	-3.785 *	0.165
1300	138.431	347.68	209.25	201.07	-4.160 *	-3.759 *	0.151
1400	142.954	362.63	219.68	202.37	-4.253 *	-3.725 *	0.139
1500	146.949	376.63	229.68	203.34	-4.443 *	-3.671 *	0.128
1600	150.496	389.78	239.28	204.04	-4.754 *	-3.620 *	0.118
1700	153.661	402.16	248.50	204.51	-5.210 *	-3.535 *	0.109
1800	156.494	413.86	257.36	204.78	-5.835 *	-3.419 *	0.099

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	17.414 kJ	MOLAR VOLUME	4.9900 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES			49.900 cm ³

SiO₂..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 313.470 - 9.47081 \times 10^{-3} T - 3.16487 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

Ca₃SiO₅ - Reference FORMULA WEIGHT 228.323

Ca₃SiO₅: Crystals 298.15 to 1800 K. Numerous small transitions occur between 298 and 1800 K in this compound.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE ELEMENTS		
					ENTHALPY	FREE ENERGY	LOG K
					GIBBS		
					kJ/mol		
298.15	0.000	168.60	168.60	171.60	-2933.137	-2787.665	488.389
UNCERTAINTY		0.31	0.31	0.86	(1.700)	(1.699)	(0.298)
400	46.672	222.31	175.64	193.35	-2932.045	-2738.068	357.557
500	77.520	267.08	189.56	207.63	-2929.979	-2689.810	281.004
600	100.112	305.90	205.79	218.02	-2927.552	-2641.985	230.006
700	117.549	340.13	222.58	225.98	-2925.149	-2594.598	193.612
800	131.511	370.74	239.22	232.30	-2925.220	-2547.261	166.320
900	143.006	398.40	255.40	237.45	-2923.225	-2500.114	145.103
1000	152.671	423.65	270.98	241.73	-2922.184	-2453.165	128.141
1100	160.936	446.86	285.93	245.35	-2922.151	-2406.289	114.266
1200	168.102	468.35	300.25	248.44	-2944.002	-2357.486	102.619
1300	174.388	488.34	313.95	251.12	-2939.505	-2308.815	92.770
1400	179.954	507.04	327.09	253.45	-2934.870	-2260.492	84.340
1500	184.923	524.60	339.67	255.49	-2930.110	-2212.473	77.046
1600	189.391	541.14	351.75	257.30	-2925.249	-2164.801	70.674
1700	193.434	556.79	363.36	258.90	-2970.804	-2116.977	65.047
1800	197.112	571.63	374.52	260.33	-3425.986	-2056.808	59.687

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	7.2742 J/bar 72.742 cm ³

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

SILICON... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 333.920 - 2.32529 \times 10^{-3} T + 2.76608 \times 10^{-5} T^2 - 6.52597 \times 10^{-8} T^3$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

32 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Ca₃SiO₅ - Reference FORMULA WEIGHT 228.323

Ca₃SiO₅: Crystals 298.15 to 1800 K. Numerous small transitions occur
between 298 and 1800 K in this compound.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	168.60	168.60	171.60	-117.156 *	-120.985 *	21.196
UNCERTAINTY		0.31	0.31	0.86	1.700	1.699	0.298
400	46.672	222.31	175.64	193.35	-117.085 *	-122.301 *	15.971
500	77.520	267.08	189.56	207.63	-116.945 *	-123.621 *	12.915
600	100.112	305.90	205.79	218.02	-116.754 *	-124.973 *	10.880
700	117.549	340.13	222.58	225.98	-116.554 *	-126.357 *	9.429
800	131.511	370.74	239.22	232.3p	-116.384 *	-127.770 *	8.343
900	143.006	398.40	255.40	237.45	-116.571 *	-129.168 *	7.497
1000	152.671	423.65	270.98	241.73	-115.512 *	-130.618 *	6.823
1100	160.936	446.86	285.93	245.35	-114.334 *	-132.187 *	6.277
1200	168.102	468.35	300.25	248.44	-113.073 *	-133.867 *	5.827
1300	174.388	488.34	313.95	251.12	-111.855 *	-135.647 *	5.450
1400	179.954	507.04	327.09	253.45	-110.445 *	-137.538 *	5.132
1500	184.923	524.60	339.67	255.49	-109.140 *	-139.510 *	4.858
1600	189.391	541.14	351.75	257.30	-107.873 *	-141.581 *	4.622
1700	193.434	556.79	363.36	258.90	-106.679 *	-143.732 *	4.416
1800	197.112	571.63	374.52	260.33	-105.563 *	-145.939 *	4.235

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	7.2742 J/bar 72.742 cm ³

TRANSITIONS IN REFERENCE STATE OXIDES

SiO₂..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 333.920 - 2.32529 \times 10^{-3} T + 2.76608 \times 10^{-3} T^{-0.5} - 6.52597 \times 10^{-4} T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

Larnite - Reference

FORMULA WEIGHT 172.244

Ca₂SiO₄: Larnite crystals 298.15 to 970 K. Alpha' crystals 970 to 1710 K. Alpha crystals 1710 to 1800 K.

TEMP. K	$(H_T^\circ - H_{298}^\circ)/T$ J/mol·K	S_T° J/mol·K	$-(G_T^\circ - H_{298}^\circ)/T$ J/mol·K	C_P° J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	126.72	126.72	128.40	-2306.697	-2191.728	383.983
UNCERTAINTY		1.29	1.29	0.24	(1.328)	(1.039)	(0.182)
400	34.960	166.95	131.99	144.97	-2306.157	-2152.484	281.087
500	58.130	200.55	142.42	156.03	-2304.876	-2114.212	220.871
600	75.157	229.76	154.60	164.19	-2303.287	-2076.214	180.751
700	88.346	255.56	167.22	170.53	-2301.659	-2038.509	152.116
800	98.950	278.68	179.73	175.64	-2301.629	-2000.843	130.642
900	107.713	299.62	191.90	179.88	-2300.177	-1963.316	113.948
970	113.015	313.19	200.17	182.45	-2299.324	-1937.070	104.312
970	114.591	314.76	200.17	179.40	-2297.796	-1937.070	104.312
1000	116.552	320.24	203.69	180.52	-2297.880	-1925.984	100.604
1100	122.545	337.63	215.09	184.49	-2297.909	-1888.811	89.693
1200	127.885	353.87	225.98	188.83	-2312.359	-1850.347	80.544
1300	132.752	369.17	236.41	193.56	-2309.006	-1812.000	72.807
1400	137.276	383.69	246.42	198.66	-2305.254	-1773.920	66.186
1500	141.548	397.59	256.04	204.14	-2301.054	-1736.101	60.457
1600	145.641	410.95	265.30	210.00	-2296.363	-1698.596	55.454
1700	149.608	423.86	274.25	216.23	-2341.643	-1660.950	51.035
1710	150.000	425.13	275.13	216.88	-2341.063	-1657.089	50.619
1710	158.415	433.55	275.13	199.60	-2326.673	-1657.089	50.619
1800	160.474	443.78	283.31	199.60	-2629.977	-1615.059	46.868

MELTING POINT	2403	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^\circ - H_0^\circ$		kJ	MOLAR VOLUME	5.1600 J/bar 51.600 cm ³

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 737, M. P. BETA 1123, E. P. 1755 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 249.689 - 2.09429 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1100 K, larnite)

$$C_P^\circ = 161.620 + 1.88970 \times 10^{-5} T^2$$

(EQUATION VALID FROM 800 - 1800 K, alpha')

$$C_P^\circ = 199.600$$

(EQUATION VALID FROM 1700 - 1800 K, alpha)

COMPILED 9-30-79

34 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Larnite - Reference

FORMULA WEIGHT 172.244

Ca₂SiO₄: Larnite crystals 298.15 to 970 K. Alpha' crystals 970
to 1710 K. Alpha crystals 1710 to 1800 K.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	126.72	126.72	128.40	-125.810 *	-128.512 *	22.515
UNCERTAINTY		1.29	1.29	0.24	1.328	1.039	0.182
400	34.960	166.95	131.99	144.97	-125.894 *	-129.420 *	16.901
500	58.130	200.55	142.42	156.03	-125.994 *	-130.292 *	13.612
600	75.157	229.76	154.60	164.19	-126.113 *	-131.141 *	11.417
700	88.346	255.56	167.22	170.53	-126.276 *	-131.966 *	9.847
800	98.950	278.68	179.73	175.64	-126.505 *	-132.764 *	8.669
900	107.713	299.62	191.90	179.88	-127.117 *	-133.496 *	7.748
970	113.015	313.19	200.17	182.45	-126.656 *	-133.900 *	7.211
970	114.591	314.76	200.17	179.40	-125.128 *	-133.900 *	7.211
1000	116.552	320.24	203.69	180.52	-125.060 *	-134.278 *	7.014
1100	122.545	337.63	215.09	184.49	-124.582 *	-135.223 *	6.421
1200	127.885	353.87	225.98	188.83	-123.889 *	-136.219 *	5.929
1300	132.752	369.17	236.41	193.56	-122.998 *	-137.281 *	5.516
1400	137.276	383.69	246.42	198.66	-121.686 *	-138.431 *	5.165
1500	141.548	397.59	256.04	204.14	-120.095 *	-139.673 *	4.864
1600	145.641	410.95	265.30	210.00	-118.123 *	-141.046 *	4.605
1700	149.608	423.86	274.25	216.23	-115.743 *	-142.555 *	4.380
1710	150.000	423.13	275.13	216.88	-115.486 *	-142.739 *	4.361
1710	158.415	433.55	275.13	199.60	-101.096 *	-142.739 *	4.361
1800	160.474	443.78	283.31	199.60	-100.337 *	-144.918 *	4.205

MELTING POINT	2403	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o		kJ	MOLAR VOLUME	5.1600 J/bar 51.600 cm ³

TRANSITIONS IN REFERENCE STATE OXIDES

SiO₂..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 249.689 - 2.09429 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1100 K, larnite)

$$C_P^o = 161.620 + 1.88970 \times 10^{-5} T^2$$

(EQUATION VALID FROM 800 - 1800 K, alpha')

$$C_P^o = 199.600$$

(EQUATION VALID FROM 1700 - 1800 K, alpha)

COMPILED 9-30-79

Larnite

FORMULA WEIGHT 172.244

Ca₂SiO₄: Crystals 298.15 to 1100K. See Larnite reference table.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^\circ - H_{298}^\circ)/T$	S_T°	$-(G_T^\circ - H_{298}^\circ)/T$	C_P°	ENTHALPY	FREE ENERGY	LOG K
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	126.72	126.72	128.40	-2306.697	-2191.728	383.983
UNCERTAINTY		1.29	1.29	0.24	(1.328)	(1.039)	(0.182)
400	34.960	166.95	131.99	144.97	-2306.157	-2152.484	281.087
500	58.130	200.55	142.42	156.03	-2304.876	-2114.212	220.871
600	75.157	229.76	154.60	164.19	-2303.287	-2076.214	180.751
700	88.346	255.56	167.22	170.53	-2301.659	-2038.509	152.116
800	98.950	278.68	179.73	175.64	-2301.629	-2000.843	130.642
900	107.713	299.62	191.90	179.88	-2300.177	-1963.316	113.948
1000	115.114	318.76	203.65	183.46	-2299.318	-1925.938	100.601
1100	121.471	336.39	214.92	186.54	-2299.090	-1888.630	89.684

MELTING POINT	2403	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ [°] - H ₀ [°]		kJ	MOLAR VOLUME	5.1600 J/bar 51.600 cm ³

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

SILICON... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 249.689 - 2.09429 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1100 K)

COMPILED 9-30-79

36 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Larnite

FORMULA WEIGHT 172.244

Ca₂SiO₄: Crystals 298.15 to 1100K. See Larnite reference table.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	126.72	126.72	128.40	-125.810 *	-128.512 *	22.515
UNCERTAINTY		1.29	1.29	0.24	1.328	1.039	0.182
400	34.960	166.95	131.99	144.97	-125.894 *	-129.420 *	16.901
500	58.130	200.55	142.42	156.03	-125.994 *	-130.292 *	13.612
600	75.157	229.76	154.60	164.19	-126.113 *	-131.141 *	11.417
700	88.346	255.56	167.22	170.53	-126.276 *	-131.966 *	9.847
800	98.950	278.68	179.73	175.64	-126.505 *	-132.764 *	8.669
900	107.713	299.62	191.90	179.88	-127.117 *	-133.496 *	7.748
1000	115.114	318.76	203.65	183.46	-126.498 *	-134.232 *	7.012
1100	121.471	336.39	214.92	186.54	-125.763 *	-135.042 *	6.413

MELTING POINT	2403	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o		kJ	MOLAR VOLUME	5.1600 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES				51.600 cm ³

SiO₂..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 249.689 - 2.09429 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1100 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

37

Calcium olivine - Reference FORMULA WEIGHT 172.244

Ca₂SiO₄: Calcium olivine crystals 298.15 to 1120 K. Alpha' crystals 1120 to 1710 K. Alpha crystals 1710 to 1800 K.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	120.50	120.50	125.69	-2316.534	-2199.710	385.382
UNCERTAINTY		2.04	2.04	0.39	(2.441)	(1.881)	(0.330)
400	33.995	159.63	125.63	140.30	-2316.380	-2159.780	282.040
500	56.348	192.11	135.76	150.85	-2315.604	-2120.720	221.551
600	72.850	220.41	147.56	159.63	-2314.508	-2081.829	181.240
700	85.794	245.59	159.80	167.07	-2313.282	-2043.156	152.463
800	96.354	268.32	171.97	173.25	-2313.543	-2004.473	130.879
900	105.181	289.02	183.84	178.14	-2312.293	-1965.897	114.098
1000	112.666	307.99	195.32	181.69	-2311.603	-1927.450	100.680
1100	119.050	325.42	206.37	183.86	-2311.590	-1889.055	89.704
1120	120.210	328.73	208.52	184.13	-2328.413	-1880.616	87.709
1120	132.441	340.96	208.52	185.32	-2314.714	-1880.616	87.709
1200	136.082	353.87	217.79	188.83	-2312.360	-1850.348	80.544
1300	140.319	369.17	228.85	193.56	-2309.006	-1811.998	72.807
1400	144.301	383.69	239.39	198.66	-2305.255	-1773.921	66.186
1500	148.106	397.59	249.48	204.14	-2301.054	-1736.101	60.457
1600	151.789	410.94	259.16	210.00	-2296.363	-1698.594	55.454
1700	155.395	423.86	268.47	216.23	-2341.643	-1660.950	51.035
1710	155.752	425.13	269.38	216.88	-2341.063	-1657.089	50.619
1710	164.167	433.55	269.38	199.60	-2326.673	-1657.089	50.619
1800	165.939	443.78	277.85	199.60	-2629.978	-1615.060	46.868

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	5.9110 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS			59.110 cm ³

CALCIUM.... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 0.106586 T - 8.15012 \times 10^{-5} T^2 + 1.65638 \times 10^{-3} T^{-0.5} - 2.36007 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 1200 K, calcium olivine)

$$C_P^o = 161.620 + 1.88970 \times 10^{-5} T^2$$

(EQUATION VALID FROM 800 - 1800 K, alpha')

$$C_P^o = 199.600$$

(EQUATION VALID FROM 1700 - 1800 K, alpha)

COMPILED 9-30-79

38 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Calcium olivine - Reference FORMULA WEIGHT 172.244

Ca₂SiO₄: Calcium olivine crystals 298.15 to 1120 K. Alpha' crystals 1120 to 1710 K. Alpha crystals 1710 to 1800 K.

TEMP. K					FORMATION FROM THE OXIDES GIBBS		
	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	120.50	120.50	125.69	-135.647 *	-136.494 *	23.913
UNCERTAINTY		2.04	2.04	0.39	2.441	1.881	0.330
400	33.995	159.63	125.63	140.30	-136.117 *	-136.717 *	17.853
500	56.348	192.11	135.76	150.85	-136.722 *	-136.800 *	14.291
600	72.850	220.41	147.56	159.63	-137.334 *	-136.756 *	11.906
700	85.794	245.59	159.80	167.07	-137.899 *	-136.613 *	10.194
800	96.354	268.32	171.97	173.25	-138.419 *	-136.394 *	8.906
900	105.181	289.02	183.84	178.14	-139.233 *	-136.076 *	7.898
1000	112.666	307.99	195.32	181.69	-138.783 *	-135.744 *	7.091
1100	119.050	325.42	206.37	183.86	-138.263 *	-135.468 *	6.433
1120	120.210	328.73	208.52	184.13	-138.162 *	-135.418 *	6.311
1120	132.441	340.96	208.52	185.32	-124.463 *	-135.418 *	6.311
1200	136.082	353.87	217.79	188.83	-123.890 *	-136.220 *	5.930
1300	140.319	369.17	228.85	193.56	-122.998 *	-137.279 *	5.516
1400	144.301	383.69	239.39	198.66	-121.687 *	-138.432 *	5.165
1500	148.106	397.59	249.48	204.14	-120.095 *	-139.673 *	4.864
1600	151.789	410.94	259.16	210.00	-118.123 *	-141.045 *	4.605
1700	155.395	423.86	268.47	216.23	-115.743 *	-142.555 *	4.380
1710	155.752	425.13	269.38	216.88	-115.486 *	-142.739 *	4.361
1710	164.167	433.55	269.38	199.60	-101.096 *	-142.739 *	4.361
1800	165.939	443.78	277.85	199.60	-100.338 *	-144.919 *	4.205

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	5.9110 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES			59.110 cm ³

SiO₂..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 106.586 T - 8.15012 \times 10^{-5} T^2 + 1.65638 \times 10^3 T^{-0.5} - 2.36007 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 200 - 1200 K, calcium olivine)

$$C_P^o = 161.620 + 1.88970 \times 10^{-5} T^2$$

(EQUATION VALID FROM 800 - 1800 K, alpha')

$$C_P^o = 199.600$$

(EQUATION VALID FROM 1700 - 1800 K, alpha)

COMPILED 9-30-79

Calcium olivine FORMULA WEIGHT 172.244

Ca₂SiO₄: Crystals 298.15 to 1200 K. See Calcium olivine reference table.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(C _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY	FREE ENERGY	LOG K
					kJ/mol	kJ/mol	
298.15	0.000	120.50	120.50	125.69	-2316.534	-2199.710	385.382
UNCERTAINTY		2.04	2.04	0.39	(2.441)	(1.881)	(0.330)
400	33.995	159.63	125.63	140.30	-2316.380	-2159.780	282.040
500	56.348	192.11	135.76	150.85	-2315.604	-2120.720	221.551
600	72.850	220.41	147.56	159.63	-2314.508	-2081.829	181.240
700	85.794	245.59	159.80	167.07	-2313.282	-2043.156	152.463
800	96.354	268.32	171.97	173.25	-2313.543	-2004.473	130.879
900	105.181	289.02	183.84	178.14	-2312.293	-1965.897	114.098
1000	112.666	307.99	195.32	181.69	-2311.603	-1927.450	100.680
1100	119.050	325.42	206.37	183.86	-2311.590	-1889.055	89.704
1200	124.492	341.46	216.97	184.62	-2326.267	-1849.363	80.501

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	5.9110 J/bar 59.110 cm ³

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM... ALPHA-BETA 737, M. P. BETA 1123, E. P. 1755 K.

SILICON... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 0.106586 T - 8.15012 \times 10^{-5} T^2 + 1.65638 \times 10^{-3} T^{-0.5} - 2.36007 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 1200 K)

COMPILED 9-30-79

40 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Calcium olivine FORMULA WEIGHT 172.244

Ca₂SiO₄: Crystals 298.15 to 1200 K. See Calcium olivine reference table.

TEMP. K	FORMATION FROM THE OXIDES GIBBS						
	(H _T ^o -H ₂₉₈ ^o)/T	S _T ^o	-(G _T ^o -H ₂₉₈ ^o)/T	C _P ^o	ENTHALPY	FREE ENERGY	LOG K
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	120.50	120.50	125.69	-135.647 *	-136.494 *	23.913
UNCERTAINTY		2.04	2.04	0.39	2.441	1.881	0.330
400	33.995	159.63	125.63	140.30	-136.117 *	-136.717 *	17.853
500	56.348	192.11	135.76	150.85	-136.722 *	-136.800 *	14.291
600	72.850	220.41	147.56	159.63	-137.334 *	-136.756 *	11.906
700	85.794	245.59	159.80	167.07	-137.899 *	-136.613 *	10.194
800	96.354	268.32	171.97	173.25	-138.419 *	-136.394 *	8.906
900	105.181	289.02	183.84	178.14	-139.233 *	-136.076 *	7.898
1000	112.666	307.99	195.32	181.69	-138.783 *	-135.744 *	7.091
1100	119.050	325.42	206.37	183.86	-138.263 *	-135.468 *	6.433
1200	124.492	341.46	216.97	184.62	-137.797 *	-135.235 *	5.887

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	5.9110 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES			59.110 cm ³
SiO ₂ ALPHA - BETA TRANSITION 844 K.			

HEAT CAPACITY EQUATION(S)

$$C_P^o = 0.106586 T - 8.15012 \times 10^{-5} T^2 + 1.65638 \times 10^{-3} T^{-0.5} - 2.36007 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 1200 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

41

Rankinite

FORMULA WEIGHT 288.408

Ca₃Si₂O₇: Crystals 298.15 to 1400 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS							
	(H _T ^o -H ₂₉₈ ^o)/T	S _T ^o	-(G _T ^o -H ₂₉₈ ^o)/T	C _P ^o	ENTHALPY	FREE ENERGY	LOG K	
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	210.60	210.60	214.37	-3985.428	-3773.475	661.100	
UNCERTAINTY		2.94	2.94	0.71	(3.200)	(2.466)	(0.432)	
400	58.460	277.87	219.41	242.56	-3984.799	-3717.493	485.457	
500	97.182	334.04	236.86	260.39	-3982.967	-3650.878	381.406	
600	125.462	382.66	257.20	272.60	-3980.721	-3584.647	312.073	
700	147.131	425.37	278.24	281.22	-3978.551	-3518.825	262.579	
800	164.299	463.35	299.05	287.39	-3978.972	-3453.013	225.460	
900	178.236	497.46	319.23	291.80	-3977.489	-3387.330	196.596	
1000	189.757	528.38	338.62	294.91	-3977.158	-3321.788	173.513	
1100	199.417	556.59	357.17	296.99	-3978.058	-3256.241	154.627	
1200	207.607	582.49	374.89	298.29	-4001.083	-3188.650	138.799	
1300	214.612	606.40	391.79	298.94	-3998.020	-3121.107	125.408	
1400	220.642	628.56	407.92	299.06	-3995.089	-3053.789	113.939	

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	9.6506 J/bar 96.506 cm ³
TRANSITIONS IN REFERENCE STATE ELEMENTS			

CALCIUM... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

SILICON... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 473.209 - 2.10355 \times 10^{-2} T + 4.31880 \times 10^3 T^{-0.5} + 3.39720 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 200 - 1400 K)

COMPILED 9-30-79

42 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Rankinite FORMULA WEIGHT 288.408

Ca₃Si₂O₇: Crystals 298.15 to 1400 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS							
	(H _T ^o -H ₂₉₈ ^o)/T	S _T ^o	-(G _T ^o -H ₂₉₈ ^o)/T	C _P ^o	ENTHALPY	FREE ENERGY	LOG K	
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol		
298.15	0.000	210.60	210.60	214.37	-258.748 *	-250.507 *	43.888	
UNCERTAINTY		2.94	2.94	0.71	3.200	2.466	0.432	
400	58.460	277.87	219.41	242.56	-258.970 *	-264.069 *	34.484	
500	97.182	334.04	236.86	260.39	-259.355 *	-265.306 *	27.716	
600	125.462	382.66	257.20	272.60	-259.997 *	-266.439 *	23.196	
700	147.131	425.37	278.24	281.22	-260.998 *	-267.437 *	19.957	
800	164.299	463.35	299.05	287.39	-262.437 *	-268.266 *	17.516	
900	178.236	497.46	319.23	291.80	-264.963 *	-268.815 *	15.602	
1000	189.757	528.38	338.62	294.91	-265.370 *	-269.217 *	14.063	
1100	199.417	556.59	357.17	296.99	-265.894 *	-269.580 *	12.801	
1200	207.607	582.49	374.89	298.29	-266.602 *	-269.886 *	11.748	
1300	214.612	606.40	391.79	298.94	-267.647 *	-270.118 *	10.854	
1400	220.642	628.56	407.92	299.06	-268.810 *	-270.275 *	10.084	

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	9.6506 J/bar 96.506 cm ³

TRANSITIONS IN REFERENCE STATE OXIDES

SiO₂..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 473.209 - 2.10355 \times 10^{-2} T + 4.31880 \times 10^3 T^{-0.5} + 3.39720 \times 10^5 T^{-2}$$

(EQUATION VALID FROM 200 - 1400 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

43

Gehlenite

FORMULA WEIGHT 274.205

Ca₂Al₂SiO₇: Crystals 298.15 to melting point 1863 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H _T ^o -H ₂₉₈ ^o)/T	S _T ^o	-(G _T ^o -H ₂₉₈ ^o)/T	C _P ^o	ENTHALPY	FREE ENERGY	LOG K
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	209.89	209.89	205.39	-3981.707	-3782.886	662.749
UNCERTAINTY		0.97	0.97	0.57	(2.458)	(2.329)	(0.408)
400	56.575	274.96	218.38	236.58	-3982.155	-3714.806	485.106
500	94.688	330.03	235.34	256.37	-3981.077	-3648.085	381.114
600	122.823	378.03	255.21	269.82	-3979.373	-3581.630	311.810
700	144.540	420.38	275.84	279.34	-3977.601	-3515.496	262.331
800	161.847	458.16	296.31	286.34	-3977.591	-3449.402	225.224
900	175.990	492.21	316.22	291.71	-3976.453	-3383.434	196.370
1000	187.786	523.17	335.39	296.05	-3997.589	-3316.032	173.212
1100	197.801	551.57	353.77	299.76	-3997.679	-3247.884	154.230
1200	206.439	577.80	371.36	303.14	-4012.323	-3178.448	138.355
1300	214.003	602.19	388.19	306.38	-4009.339	-3109.075	124.925
1400	220.718	625.01	404.30	309.66	-4006.178	-3039.975	113.423
1500	226.761	646.49	419.73	313.10	-4002.802	-2971.060	103.462
1600	232.271	666.82	434.55	316.80	-3999.190	-2902.409	94.754
1700	237.360	686.14	448.78	320.82	-4045.800	-2833.561	87.065
1800	242.118	704.60	462.49	325.24	-4348.290	-2755.625	79.966

MELTING POINT	1863	K	BOILING POINT		K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION		kJ
H ₂₉₈ ^o - H ₀ ^o		kJ	MOLAR VOLUME		9.0240 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS					90.240 cm ³

CALCIUM... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

ALUMINUM... M. P. 933 K.

SILICON... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_p^o = 588.351 - 6.71533 \times 10^{-2} T + 3.89086 \times 10^{-5} T^2 - 6.27433 \times 10^{-3} T^{-0.5} + 1.51047 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

44 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Gehlenite

FORMULA WEIGHT 274.205

Ca₂Al₂SiO₇: Crystals 298.15 to melting point 1863 K.

TEMP. K	FORMATION FROM THE OXIDES GIBBS						
	(H _T ^o -H ₂₉₈ ^o)/T	S _T ^o	-(G _T ^o -H ₂₉₈ ^o)/T	C _P ^o	ENTHALPY	FREE ENERGY	LOG K
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	209.89	209.89	205.39	-125.109 *	-137.428 *	24.077
UNCERTAINTY		0.97	0.97	0.57	2.458	2.329	0.408
400	56.575	274.96	218.38	236.58	-125.529 *	-141.574 *	18.488
500	94.688	330.03	235.34	256.37	-126.086 *	-145.525 *	15.203
600	122.823	378.03	255.21	269.82	-126.793 *	-149.349 *	13.002
700	144.540	420.38	275.84	279.34	-127.697 *	-153.039 *	11.420
800	161.847	458.16	296.31	286.34	-128.832 *	-156.585 *	10.224
900	175.990	492.21	316.22	291.71	-130.506 *	-159.940 *	9.283
1000	187.786	523.17	335.39	296.05	-131.095 *	-163.176 *	8.523
1100	197.801	551.57	353.77	299.76	-131.687 *	-166.357 *	7.900
1200	206.439	577.80	371.36	303.14	-132.284 *	-169.482 *	7.377
1300	214.003	602.19	388.19	306.38	-132.937 *	-172.555 *	6.933
1400	220.718	625.01	404.30	309.66	-133.454 *	-175.590 *	6.551
1500	226.761	646.49	419.73	313.10	-133.993 *	-178.570 *	6.218
1600	232.271	666.82	434.55	316.80	-134.467 *	-181.532 *	5.926
1700	237.360	686.14	448.78	320.82	-134.855 *	-184.466 *	5.668
1800	242.118	704.60	462.49	325.24	-135.112 *	-187.373 *	5.437

MELTING POINT	1863	K	BOILING POINT	K
ENTHALPY OF MELTING		kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o		kJ	MOLAR VOLUME	9.0240 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES				90.240 cm ³
SiO ₂ ALPHA - BETA TRANSITION 844 K.				

HEAT CAPACITY EQUATION(S)

$$C_P^o = 588.351 - 6.71533 \times 10^{-2} T + 3.89086 \times 10^{-5} T^2 - 6.27433 \times 10^{-3} T^{-0.5} + 1.51047 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

45

Grossular

FORMULA WEIGHT 450.454

Ca₃Al₂Si₃O₁₂: Crystals 298.15 to 1400 K.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(C _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	255.97	255.97	330.51	-6636.338 (3.220)	-6274.723 (2.583)	1099.310 (0.453)
400	92.227	361.99	269.76	389.09	-6637.014	-6150.923	803.232
500	155.482	452.99	297.51	425.32	-6634.725	-6029.647	629.916
600	202.582	532.80	330.22	449.24	-6631.123	-5908.932	514.421
700	239.046	603.34	364.30	465.39	-6627.209	-5788.899	431.975
800	268.070	666.25	398.18	476.38	-6625.827	-5669.117	370.157
900	291.657	722.82	431.16	483.83	-6622.715	-5549.686	322.097
1000	311.138	774.07	462.93	488.77	-6642.389	-5429.040	283.585
1100	327.442	820.82	493.37	491.93	-6641.628	-5307.775	252.046
1200	341.236	863.71	522.47	493.83	-6663.054	-5184.609	225.681
1300	353.016	903.28	550.26	494.83	-6658.468	-5061.614	203.379
1400	363.162	939.97	576.81	495.21	-6654.095	-4938.997	184.277

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	47.047 kJ	MOLAR VOLUME	12.5300 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS			125.300 cm ³

CALCIUM... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

ALUMINUM... M. P. 933 K.

SILICON... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 985.362 - 9.66435 \times 10^{-2} T + 3.35314 \times 10^{-5} T^2 - 1.07077 \times 10^{-4} T^{-0.5} + 1.77080 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 200 - 1400 K)

COMPILED 9-30-79

46 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Crossular

FORMULA WEIGHT 450.454

Ca₃Al₂Si₃O₁₂: Crystals 298.15 to 1400 K.

TEMP. K					FORMATION FROM THE OXIDES GIBBS		
	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	255.97	255.97	330.51	-323.248 *	-313.225 *	54.876
UNCERTAINTY		2.95	2.95	0.15	3.220	2.583	0.453
400	92.227	361.99	269.76	389.09	-323.953 *	-309.675 *	40.440
500	155.482	452.99	297.51	425.32	-324.426 *	-306.053 *	31.973
600	202.582	532.80	330.22	449.24	-325.067 *	-302.322 *	26.320
700	239.046	603.34	364.30	465.39	-326.176 *	-298.449 *	22.271
800	268.070	666.25	398.18	476.38	-327.957 *	-294.378 *	19.221
900	291.657	722.82	431.16	483.83	-331.430 *	-289.929 *	16.827
1000	311.138	774.07	462.93	488.77	-331.811 *	-285.295 *	14.902
1100	327.442	820.82	493.37	491.93	-332.452 *	-280.617 *	13.325
1200	341.236	863.71	522.47	493.83	-333.452 *	-275.861 *	12.008
1300	353.016	903.28	550.26	494.83	-334.977 *	-271.005 *	10.889
1400	363.162	939.97	576.81	495.21	-336.806 *	-266.028 *	9.926

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	47.047 kJ	MOLAR VOLUME	12.5300 J/bar 125.300 cm ³
TRANSITIONS IN REFERENCE STATE OXIDES			
SiO ₂ ALPHA - BETA TRANSITION 844 K.			

HEAT CAPACITY EQUATION(S)

$$C_P^o = 985.362 - 9.66435 \times 10^{-2} T + 3.35314 \times 10^{-5} T^2 - 1.07077 \times 10^{-4} T^{-0.5} + 1.77080 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 1400 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

47

Zoisite

FORMULA WEIGHT 454.363

Ca₂Al₃Si₃O₁₂(OH): Crystals 298.15 to 900 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						LOG K
	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	
298.15	0.000	295.88	295.88	350.86	-6891.117	-6495.296	1137.954
UNCERTAINTY		0.72	0.72	0.48	(2.080)	(2.022)	(0.354)
400	97.635	408.13	310.50	411.31	-6892.551	-6359.695	830.495
500	164.514	504.38	339.86	450.35	-6890.830	-6226.657	650.497
600	214.590	589.07	374.48	478.14	-6887.457	-6094.097	530.541
700	253.787	664.41	410.62	498.85	-6883.311	-5962.212	444.908
800	285.456	732.10	446.65	514.77	-6880.441	-5830.734	380.710
900	311.657	793.49	481.83	526.28	-6876.128	-5699.747	330.806

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	13.6520 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS			136.520 cm ³

CALCIUM.... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 834.622 - 1.98447 \times 10^{-2} T + 8.14875 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 900 K)

COMPILED 9-30-79

48 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Zoisite

FORMULA WEIGHT 454.363

$\text{Ca}_2\text{Al}_3\text{Si}_3\text{O}_{12}(\text{OH})$: Crystals 298.15 to 900 K.

TEMP. K	$(H_T^\circ - H_{298}^\circ)/T$ J/mol·K	S_T° J/mol·K	$-(G_T^\circ - H_{298}^\circ)/T$ J/mol·K	C_P° J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	295.88	295.88	350.86	-232.361 *	-227.585 *	39.872
UNCERTAINTY		0.72	0.72	0.48	2.080	2.022	0.354
400	97.635	408.13	310.50	411.31	-254.577 *	-224.110 *	29.266
500	164.514	504.38	339.86	450.35	-254.706 *	-216.481 *	22.616
600	214.590	589.07	374.48	478.14	-254.929 *	-208.815 *	18.179
700	253.787	664.41	410.62	498.85	-255.399 *	-201.093 *	15.006
800	285.456	732.10	446.65	514.77	-256.230 *	-193.288 *	12.620
900	311.657	793.49	481.83	526.28	-258.387 *	-185.243 *	10.751

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^\circ - H_0^\circ$	kJ	MOLAR VOLUME	13.6520 J/bar 136.520 cm^3

TRANSITIONS IN REFERENCE STATE OXIDES

SiO_2 ALPHA - BETA TRANSITION 844 K.

H_2O B. P. 372.8 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 834.622 - 1.98447 \times 10^{-2} T - 8.14875 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 900 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

49

CaSiO₃ - Reference FORMULA WEIGHT 116.164

CaSiO₃: Wollastonite crystals 298.15 to 1398 K. Cyclo wollastonite is the stable phase above 1398 K.

TEMP. K	$(H_T^\circ - H_{298}^\circ)/T$				FORMATION FROM THE ELEMENTS GIBBS		
	S_T°	$-(C_T^\circ - H_{298}^\circ)/T$	C_p°	ENTHALPY	FREE ENERGY	LOG K	
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	81.03	81.03	87.56	-1634.766	-1549.164	271.408
UNCERTAINTY		0.68	0.68	0.55	(0.702)	(0.608)	(0.107)
400	23.967	108.60	84.63	99.71	-1634.490	-1519.929	198.483
500	39.936	131.73	91.80	107.41	-1633.684	-1491.381	155.804
600	51.657	151.82	100.17	112.81	-1632.658	-1463.006	127.367
700	60.691	169.53	108.83	116.80	-1631.593	-1434.821	107.068
800	67.904	185.33	117.43	119.86	-1631.334	-1406.691	91.848
900	73.817	199.59	125.78	122.29	-1630.382	-1378.657	80.016
1000	78.766	212.58	133.82	124.26	-1629.752	-1350.726	70.555
1100	82.979	224.51	141.53	125.91	-1629.467	-1322.850	62.817
1200	86.617	235.52	148.91	127.32	-1636.486	-1294.342	56.341
1300	89.796	245.76	155.97	128.56	-1634.731	-1265.915	50.865
1398	92.553	255.15	162.60	129.65	-1632.970	-1238.183	46.263
1398	96.691	259.29	162.60	129.53	-1627.185	-1238.183	46.263
1400	96.738	259.47	162.73	129.56	-1627.150	-1237.632	46.177
1500	98.965	268.45	169.49	130.73	-1625.31P	-1209.863	42.131
1600	100.984	276.92	175.94	131.78	-1623.436	-1182.233	38.596
1700	102.825	284.94	182.12	132.73	-1672.018	-1154.277	35.467
1800	104.511	292.55	188.04	133.60	-1823.266	-1120.516	32.517

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	3.9930 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS			39.930 cm ³

CALCIUM.... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_p^\circ = 192.773 - 9.11511 \times 10^{-3} T + 4.41319 \times 10^{-6} T^2 - 1.72960 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1500 K, wollastonite)

$$C_p^\circ = 167.255 - 3.62159 \times 10^{-4} T - 1.37237 \times 10^{-3} T^{-0.5} - 9.73908 \times 10^{-3} T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K, cyclo wollastonite)

COMPILED 9-30-79

CaSiO₃ - Reference

FORMULA WEIGHT 116.164

CaSiO₃: Wollastonite crystals 298.15 to 1398 K. Cyclo wollastonite is the stable phase above 1398 K.

TEMP. K	$(H_T^{\circ} - H_{298}^{\circ})/T$ J/mol·K	S_T° J/mol·K	$-(G_T^{\circ} - H_{298}^{\circ})/T$ J/mol·K	C_P° J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	81.03	81.03	87.56	-88.973 *	-89.412 *	15.665
UNCERTAINTY		0.68	0.68	0.55	0.702	0.608	0.107
400	23.967	108.60	84.63	99.71	-88.924 *	-89.569 *	11.697
500	39.936	131.73	91.80	107.41	-88.954 *	-89.729 *	9.374
600	51.657	151.82	100.17	112.81	-89.108 *	-89.872 *	7.824
700	60.691	169.53	108.83	116.80	-89.423 *	-89.976 *	6.714
800	67.904	185.33	117.43	119.86	-89.923 *	-90.024 *	5.878
900	73.817	199.59	125.78	122.29	-90.916 *	-89.962 *	5.221
1000	78.766	212.58	133.82	124.26	-90.784 *	-89.861 *	4.694
1100	82.979	224.51	141.53	125.91	-90.630 *	-89.777 *	4.263
1200	86.617	235.52	148.91	127.32	-90.475 *	-89.705 *	3.905
1300	89.796	245.76	155.97	128.56	-90.366 *	-89.646 *	3.602
1398	92.553	255.15	162.60	129.65	-90.224 *	-89.596 *	3.348
1398	96.691	259.29	162.60	129.53	-84.439 *	-89.596 *	3.348
1400	96.738	259.47	162.73	129.56	-84.439 *	-89.607 *	3.343
1500	98.965	268.45	169.49	130.73	-84.370 *	-89.970 *	3.133
1600	100.984	276.92	175.94	131.78	-84.333 *	-90.353 *	2.950
1700	102.825	284.94	182.12	132.73	-84.344 *	-90.731 *	2.788
1800	104.511	292.55	188.04	133.60	-84.408 *	-91.103 *	2.644

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^{\circ} - H_0^{\circ}$	kJ	MOLAR VOLUME	3.9930 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES			39.930 cm ³
SiO ₂ ALPHA - BETA TRANSITION	844 K.		

HEAT CAPACITY EQUATION(S)

$$C_P^{\circ} = 192.773 - 9.11511 \times 10^{-3} T + 4.41319 \times 10^{-6} T^2 - 1.72960 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1500 K, wollastonite)

$$C_P^{\circ} = 167.255 - 3.62159 \times 10^{-4} T - 1.37237 \times 10^{-3} T^{-0.5} - 9.73908 \times 10^{-3} T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K, cyclo wollastonite)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

51

Wollastonite

FORMULA WEIGHT 116.164

CaSiO₃: Crystals 298.15 to 1500 K. See CaSiO₃ reference table.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS			C _p J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K				
298.15	0.000	81.03	81.03	87.56	-1634.766	-1549.164	271.408
UNCERTAINTY		0.68	0.68	0.55	(0.702)	(0.608)	(0.107)
400	23.967	108.60	84.63	99.71	-1634.490	-1519.929	198.483
500	39.936	131.73	91.80	107.41	-1633.684	-1491.381	155.804
600	51.657	151.82	100.17	112.81	-1632.658	-1463.006	127.367
700	60.691	169.53	108.83	116.80	-1631.593	-1434.821	107.068
800	67.904	185.33	117.43	119.86	-1631.334	-1406.691	91.848
900	73.817	199.59	125.78	122.29	-1630.382	-1378.657	80.016
1000	78.766	212.58	133.82	124.26	-1629.752	-1350.726	70.555
1100	82.979	224.51	141.53	125.91	-1629.467	-1322.850	62.817
1200	86.617	235.52	148.91	127.32	-1636.486	-1294.342	56.341
1300	89.796	245.76	155.97	128.56	-1634.731	-1265.915	50.865
1400	92.606	255.33	162.73	129.67	-1632.935	-1237.623	46.176
1500	95.112	264.32	169.20	130.70	-1631.098	-1209.441	42.117

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	3.9930 J/bar 39.930 cm ³

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_p^o = 192.773 - 9.11511 \times 10^{-3} T + 4.41319 \times 10^{-6} T^2 - 1.72960 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1500 K)

COMPILED 9-30-79

52 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Wollastonite

FORMULA WEIGHT 116.164

CaSiO₃: Crystals 298.15 to 1500 K. See CaSiO₃ reference table.

TEMP. K	$(H_T^\circ - H_{298}^\circ)/T$ J/mol·K	S_T° J/mol·K	$-(G_T^\circ - H_{298}^\circ)/T$ J/mol·K	C_P° J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	81.03	81.03	87.56	-88.973 *	-89.412 *	15.665
UNCERTAINTY		0.68	0.68	0.55	0.702	0.608	0.107
400	23.967	108.60	84.63	99.71	-88.924 *	-89.569 *	11.697
500	39.936	131.73	91.80	107.41	-88.954 *	-89.729 *	9.374
600	51.657	151.82	100.17	112.81	-89.108 *	-89.872 *	7.824
700	60.691	169.53	108.83	116.80	-89.423 *	-89.976 *	6.714
800	67.904	185.33	117.43	119.86	-89.923 *	-90.024 *	5.878
900	73.817	199.59	125.78	122.29	-90.916 *	-89.962 *	5.221
1000	78.766	212.58	133.82	124.26	-90.784 *	-89.861 *	4.694
1100	82.979	224.51	141.53	125.91	-90.630 *	-89.777 *	4.263
1200	86.617	235.52	148.91	127.32	-90.475 *	-89.705 *	3.905
1300	89.796	245.76	155.97	128.56	-90.366 *	-89.646 *	3.602
1400	92.606	255.33	162.73	129.67	-90.224 *	-89.599 *	3.343
1500	95.112	264.32	169.20	130.70	-90.150 *	-89.547 *	3.118

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^\circ - H_0^\circ$	kJ	MOLAR VOLUME	3.9930 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES			39.930 cm ³
SiO ₂ ALPHA - BETA TRANSITION 844 K.			

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 192.773 - 9.11511 \times 10^{-3} T + 4.41319 \times 10^{-6} T^2 - 1.72960 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1500 K)

COMPILED 9-30-79

Cyclo wollastonite (Pseudowollastonite)

FORMULA WEIGHT 116.164

CaSiO₃: Crystals 298.15 to 1800 K. See CaSiO₃ reference table.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H _T [°] -H ₂₉₈ [°])/T	S _T [°]	-(G _T [°] -H ₂₉₈ [°])/T	C _P [°]	ENTHALPY	FREE ENERGY	LOG K
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	87.24	87.24	87.45	-1627.614	-1543.865	270.480
UNCERTAINTY		0.91	0.91	1.55	(0.932)	(0.784)	(0.137)
400	23.750	114.57	90.82	98.29	-1627.425	-1515.253	197.873
500	39.416	137.32	97.91	105.48	-1626.792	-1487.284	155.376
600	50.888	157.05	106.16	110.77	-1625.967	-1459.449	127.057
700	59.746	174.44	114.69	114.86	-1625.103	-1431.771	106.840
800	66.846	190.00	123.15	118.14	-1625.028	-1404.120	91.680
900	72.701	204.08	131.37	120.84	-1624.234	-1376.542	79.893
1000	77.632	216.93	139.30	123.12	-1623.734	-1349.052	70.468
1100	81.858	228.76	146.90	125.07	-1623.548	-1321.606	62.758
1200	85.532	239.71	154.18	126.76	-1630.636	-1293.520	56.306
1300	88.762	249.92	161.16	128.24	-1628.924	-1265.510	50.849
1400	91.629	259.47	167.84	129.56	-1627.150	-1237.633	46.177
1500	94.198	268.45	174.25	130.73	-1625.317	-1209.864	42.131
1600	96.514	276.92	180.41	131.78	-1623.436	-1182.233	38.596
1700	98.618	284.94	186.32	132.73	-1672.018	-1154.278	35.467
1800	100.537	292.55	192.02	133.60	-1823.266	-1120.518	32.517

MELTING POINT	1817	K	BOILING POINT	K
ENTHALPY OF MELTING	27.405	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ [°] - H ₀ [°]		kJ	MOLAR VOLUME	4.0080 J/bar 40.080 cm ³

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM.... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 167.255 - 3.62159 \times 10^{-4} T + 1.37237 \times 10^{-3} T^{-0.5} - 9.73908 \times 10^{-3} T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

54 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Cyclo wollastonite (Pseudowollastonite)

FORMULA WEIGHT 116.164

CaSiO₃: Crystals 298.15 to 1800 K. See CaSiO₃ reference table.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	87.24	87.24	87.45	-81.821 *	-84.113 *	14.736
UNCERTAINTY		0.91	0.91	1.55	0.932	0.784	0.137
400	23.750	114.57	90.82	98.29	-81.859 *	-84.893 *	11.086
500	39.416	137.32	97.91	105.48	-82.062 *	-85.633 *	8.946
600	50.888	157.05	106.16	110.77	-82.417 *	-86.315 *	7.514
700	59.746	174.44	114.69	114.86	-82.933 *	-86.926 *	6.486
800	66.846	190.00	123.15	118.14	-83.617 *	-87.453 *	5.710
900	72.701	204.08	131.37	120.84	-84.768 *	-87.847 *	5.099
1000	77.632	216.93	139.30	123.12	-84.766 *	-88.187 *	4.606
1100	81.858	228.76	146.90	125.07	-84.711 *	-88.533 *	4.204
1200	85.532	239.71	154.18	126.76	-84.625 *	-88.883 *	3.869
1300	88.762	249.92	161.16	128.24	-84.559 *	-89.241 *	3.586
1400	91.629	259.47	167.84	129.56	-84.439 *	-89.609 *	3.343
1500	94.198	268.45	174.25	130.73	-84.369 *	-89.970 *	3.133
1600	96.514	276.92	180.41	131.78	-84.333 *	-90.353 *	2.950
1700	98.618	284.94	186.32	132.73	-84.344 *	-90.733 *	2.788
1800	100.537	292.55	192.02	133.60	-84.408 *	-91.105 *	2.644

MELTING POINT	1817	K	BOILING POINT	K
ENTHALPY OF MELTING	27.405	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o		kJ	MOLAR VOLUME	4.0080 J/bar 40.080 cm ³
TRANSITIONS IN REFERENCE STATE OXIDES				
SiO ₂ ALPHA - BETA TRANSITION 844 K.				

HEAT CAPACITY EQUATION(S)

$$C_P^o = 167.255 - 3.62159 \times 10^{-4} T + 1.37237 \times 10^{-3} T^{-0.5} - 9.73908 \times 10^{-3} T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

Ca-Al pyroxene

FORMULA WEIGHT 218.125

CaAl₂SiO₆: Crystals 298.15 to 1800 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^\circ - H_{298}^\circ)/T$	S_T°	$-(G_T^\circ - H_{298}^\circ)/T$	C_P°	ENTHALPY	FREE ENERGY	LOG K
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	141.61	141.61	165.66	-3298.956	-3122.767	547.098
UNCERTAINTY		2.17	2.17	2.74	(1.912)	(1.468)	(0.257)
400	46.527	195.09	148.56	196.56	-3299.290	-3062.442	399.916
500	78.432	240.99	162.56	214.22	-3298.096	-3003.358	313.760
600	102.107	281.16	179.05	226.06	-3296.254	-2944.570	256.349
700	120.459	316.69	196.23	234.68	-3294.215	-2886.126	215.366
800	135.169	348.47	213.31	241.32	-3292.983	-2827.867	184.642
900	147.268	377.22	229.95	246.63	-3291.181	-2769.826	160.757
1000	157.429	403.43	246.00	251.01	-3311.212	-2710.445	141.580
1100	166.108	427.53	261.43	254.69	-3309.757	-2650.443	125.860
1200	173.626	449.83	276.21	257.86	-3315.484	-2589.936	112.737
1300	180.214	470.59	290.37	260.61	-3312.328	-2529.593	101.641
1400	186.045	489.99	303.95	263.04	-3309.043	-2469.534	92.140
1500	191.251	508.21	316.96	265.20	-3305.637	-2409.674	83.913
1600	195.935	525.39	329.46	267.14	-3302.131	-2350.068	76.722
1700	200.176	541.64	341.46	268.89	-3349.037	-2290.259	70.371
1800	204.039	557.06	353.02	270.49	-3498.565	-2224.700	64.559

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^\circ - H_0^\circ$	kJ	MOLAR VOLUME	6.3500 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS			63.500 cm ³

CALCIUM.... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 322.848 - 2.18582 \times 10^3 T^{-0.5} - 2.72024 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

Ca-Al pyroxene

FORMULA WEIGHT 218.125

CaAl₂SiO₆: Crystals 298.15 to 1800 K.

TEMP. K	$(H_T^\circ - H_{298}^\circ)/T$ J/mol·K	S_T° J/mol·K	$-(C_T^\circ - H_{298}^\circ)/T$ J/mol·K	C_P° J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	141.61	141.61	165.66	-77.452 *	-80.773 *	14.151
UNCERTAINTY		2.17	2.17	2.74	1.912	1.468	0.257
400	46.527	195.09	148.56	196.56	-77.361 *	-81.914 *	10.697
500	78.432	240.99	162.56	214.22	-77.257 *	-83.067 *	8.678
600	102.107	281.16	179.05	226.06	-77.298 *	-84.227 *	7.333
700	120.459	316.69	196.23	234.68	-77.523 *	-85.367 *	6.370
800	135.169	348.47	213.31	241.32	-77.936 *	-86.462 *	5.645
900	147.268	377.22	229.95	246.63	-78.828 *	-87.458 *	5.076
1000	157.429	403.43	246.00	251.01	-78.570 *	-88.430 *	4.619
1100	166.108	427.53	261.43	254.69	-78.255 *	-89.431 *	4.247
1200	173.626	449.83	276.21	257.86	-77.904 *	-90.461 *	3.938
1300	180.214	470.59	290.37	260.61	-77.568 *	-91.522 *	3.677
1400	186.045	489.99	303.95	263.04	-77.176 *	-92.614 *	3.455
1500	191.251	508.21	316.96	265.20	-76.839 *	-93.719 *	3.264
1600	195.935	525.39	329.46	267.14	-76.544 *	-94.862 *	3.097
1700	200.176	541.64	341.46	268.89	-76.317 *	-96.014 *	2.950
1800	204.039	557.06	353.02	270.49	-76.170 *	-97.177 *	2.820

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^\circ - H_0^\circ$	kJ	MOLAR VOLUME	6.3500 J/bar 63.500 cm ³

TRANSITIONS IN REFERENCE STATE OXIDES

SiO₂..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 322.848 - 2.18582 \times 10^3 T^{-0.5} - 2.72024 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

57

Anorthite

FORMULA WEIGHT 278.210

CaAl₂Si₂O₈: Crystals 298.15 to melting point 1830 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H _T ^o -H ₂₉₈ ^o)/T	S _T ^o	-(G _T ^o -H ₂₉₈ ^o)/T	C _p ^o	ENTHALPY	FREE ENERGY	LOG K
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	199.29	199.29	211.60	-4227.833	-4002.070	701.149
UNCERTAINTY		0.14	0.14	0.15	(1.118)	(1.117)	(0.196)
400	58.887	266.99	208.10	248.14	-4228.401	-3924.761	512.523
500	99.194	325.01	225.81	271.07	-4227.120	-3848.987	402.103
600	129.192	375.87	246.67	286.33	-4224.968	-3773.543	328.518
700	152.447	420.85	268.40	297.05	-4222.519	-3698.508	275.987
800	171.049	461.07	290.02	305.15	-4220.847	-3623.718	236.606
900	186.331	497.41	311.08	311.89	-4218.581	-3549.197	205.991
1000	199.199	530.59	331.39	318.09	-4238.088	-3473.399	181.433
1100	210.289	561.20	350.91	324.34	-4235.980	-3397.041	161.313
1200	220.069	589.70	369.63	331.06	-4240.825	-3320.228	144.526
1300	228.891	616.49	387.60	338.57	-4236.439	-3243.686	130.333
1400	237.022	641.89	404.87	347.08	-4231.443	-3167.541	118.183
1500	244.675	666.16	421.48	356.78	-4225.699	-3091.723	107.664
1600	252.020	689.53	437.51	367.83	-4219.071	-3016.348	98.474
1700	259.192	712.20	453.00	380.32	-4312.415	-2940.560	90.353
1800	266.304	734.33	468.02	394.35	-4456.468	-2856.728	82.900

MELTING POINT	1830	K	BOILING POINT	K
ENTHALPY OF MELTING	81.000	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	33.333	kJ	MOLAR VOLUME	10.0790 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS				100.790 cm ³

CALCIUM.... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_p^o = 800.971 - 0.146450 T + 1.05663 \times 10^{-4} T^2 - 9.44981 \times 10^{-8} T^{-0.5} + 3.18591 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

58 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Anorthite

FORMULA WEIGHT 278.210

CaAl₂Si₂O₈: Crystals 298.15 to melting point 1830 K.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	199.29	199.29	211.60	-95.630 *	-103.788 *	18.183
UNCERTAINTY		0.14	0.14	0.15	1.118	1.117	0.196
400	58.887	266.99	208.10	248.14	-95.603 *	-106.576 *	13.918
500	99.194	325.01	225.81	271.07	-95.703 *	-109.313 *	11.420
600	129.192	375.87	246.67	286.33	-96.086 *	-112.005 *	9.751
700	152.447	420.85	268.40	297.05	-96.869 *	-114.601 *	8.552
800	171.049	461.07	290.02	305.15	-98.101 *	-117.058 *	7.643
900	186.331	497.41	311.08	311.89	-100.356 *	-119.260 *	6.922
1000	199.199	530.59	331.39	318.09	-100.330 *	-121.360 *	6.339
1100	210.289	561.20	350.91	324.34	-100.131 *	-123.471 *	5.863
1200	220.069	589.70	369.63	331.06	-99.693 *	-125.608 *	5.468
1300	228.891	616.49	387.60	338.57	-98.956 *	-127.796 *	5.135
1400	237.022	641.89	404.87	347.08	-97.722 *	-130.061 *	4.853
1500	244.675	666.16	421.48	356.78	-95.964 *	-132.409 *	4.611
1600	252.020	689.53	437.51	367.83	-93.517 *	-134.932 *	4.405
1700	259.192	712.20	453.00	380.32	-90.246 *	-137.619 *	4.229
1800	266.304	734.33	468.02	394.35	-85.998 *	-140.520 *	4.078

MELTING POINT	1830	K	BOILING POINT	K
ENTHALPY OF MELTING	81.000	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	33.333	kJ	MOLAR VOLUME	10.0790 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES				100.790 cm ³

SiO₂..... ALPHA - BETA TRANSITION 844 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 800.971 - 0.146450 T + 1.05663 \times 10^{-4} T^2 - 9.44981 \times 10^3 T^{-0.5} + 3.18591 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 200 - 1800 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

59

Kaolinite

FORMULA WEIGHT 258.161

$Al_2Si_2O_5(OH)_4$: Crystals 298.15 to 1000 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	$(H_T^\circ - H_{298}^\circ)/T$	S_T°	$-(G_T^\circ - H_{298}^\circ)/T$	C_P°	ENTHALPY	FREE ENERGY	LOG K
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	204.97	204.97	246.14	-4119.780	-3799.611	665.679
UNCERTAINTY		1.02	1.02	0.77	(1.065)	(0.982)	(0.172)
400	68.780	284.03	215.25	290.40	-4121.208	-3689.902	481.854
500	115.990	351.94	235.95	317.20	-4120.173	-3582.177	374.229
600	151.042	411.38	260.34	334.09	-4117.887	-3474.764	302.506
700	178.000	463.74	285.74	344.52	-4115.089	-3367.809	251.310
800	199.226	510.17	310.94	350.48	-4112.291	-3261.240	212.938
900	216.209	551.63	335.43	353.18	-4109.855	-3154.980	183.111
1000	229.937	588.88	358.94	353.45	-4129.370	-3047.479	159.185

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^\circ - H_0^\circ$	kJ	MOLAR VOLUME	9.9520 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS			99.520 cm ³

ALUMINUM... M. P. 933 K.

SILICON.... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 749.175 - 6.77102 \times 10^{-2} T - 8.27864 \times 10^{-3} T^{-0.5} + 1.49195 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 1000 K)

COMPILED 9-30-79

60 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Kaolinite FORMULA WEIGHT 258.161

Al₂Si₂O₅(OH)₄: Crystals 298.15 to 1000 K.

TEMP. K	(H _T [°] -H ₂₉₈ [°])/T J/mol·K	S _T [°] J/mol·K	-(G _T [°] -H ₂₉₈ [°])/T J/mol·K	C _P [°] J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY	FREE ENERGY	LOG K
					kJ/mol	kJ/mol	
298.15	0.000	204.97	204.97	246.14	-51.055 *	-30.571 *	5.356
UNCERTAINTY		1.02	1.02	0.77	1.065	0.982	0.172
400	68.780	284.03	215.25	290.40	-137.391 *	-16.597 *	2.167
500	115.990	351.94	235.95	317.20	-135.216 *	13.350 *	-1.395
600	151.042	411.38	260.34	334.09	-133.059 *	42.862 *	-3.731
700	178.000	463.74	285.74	344.52	-131.327 *	72.043 *	-5.376
800	199.226	510.17	310.94	350.48	-130.314 *	101.007 *	-6.595
900	216.209	551.63	335.43	353.18	-130.802 *	129.974 *	-7.544
1000	229.937	588.88	358.94	353.45	-129.698 *	158.885 *	-8.299

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ [°] - H ₀ [°]	kJ	MOLAR VOLUME	9.9520 J/bar 99.520 cm ³

TRANSITIONS IN REFERENCE STATE OXIDES

SiO₂..... ALPHA - BETA TRANSITION 844 K.

H₂O..... B. P. 372.8 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 749.175 - 6.77102 \times 10^{-2} T - 8.27864 \times 10^3 T^{-0.5} + 1.49195 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 200 - 1000 K)

COMPILED 9-30-79

Dickite

FORMULA WEIGHT 258.161

$Al_2Si_2O_5(OH)_4$: Crystals 298.15 to 900 K.

TEMP. K	$(H_T^\circ - H_{298}^\circ)/T$ J/mol·K	S_T° J/mol·K	$-(G_T^\circ - H_{298}^\circ)/T$ J/mol·K	C_P° J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY	FREE ENERGY	LOG K
					kJ/mol	kJ/mol	
298.15	0.000	197.06	197.06	239.79	-4118.475	-3795.948	665.037
UNCERTAINTY		3.07	3.07	0.74	(1.237)	(1.538)	(0.269)
400	67.647	274.79	207.14	287.84	-4120.356	-3685.353	481.260
500	114.860	342.44	227.58	317.24	-4119.433	-3576.686	373.655
600	150.208	402.00	251.79	335.08	-4117.082	-3468.326	301.946
700	177.410	454.48	277.07	345.05	-4114.198	-3360.439	250.760
800	198.688	500.90	302.21	349.43	-4111.417	-3252.946	212.397
900	215.484	542.10	326.62	349.69	-4109.202	-3145.747	182.575

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^\circ - H_0^\circ$	kJ	MOLAR VOLUME	9.9300 J/bar 99.300 cm ³
TRANSITIONS IN REFERENCE STATE ELEMENTS			
ALUMINUM... M. P. 933 K.			
SILICON... M. P. 1685 K.			

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 908.360 - 0.105663 T - 1.11953 \times 10^4 T^{-0.5} + 3.80445 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 200 - 900 K)

COMPILED 9-30-79

62 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Dickite

FORMULA WEIGHT 258.161

$Al_2Si_2O_5(OH)_4$: Crystals 298.15 to 900 K.

TEMP. K	$(H_T^\circ - H_{298}^\circ)/T$ J/mol·K	S_T° J/mol·K	$-(G_T^\circ - H_{298}^\circ)/T$ J/mol·K	C_P° J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	197.06	197.06	239.79	-49.750 *	-26.908 *	4.714
UNCERTAINTY		3.07	3.07	0.74	1.237	1.538	0.269
400	67.647	274.79	207.14	287.84	-136.539 *	-12.048 *	1.573
500	114.860	342.44	227.58	317.24	-134.476 *	18.842 *	-1.968
600	150.208	402.00	251.79	335.08	-132.254 *	49.299 *	-4.292
700	177.410	454.48	277.07	345.05	-130.435 *	79.413 *	-5.926
800	198.688	500.90	302.21	349.43	-129.440 *	109.301 *	-7.137
900	215.484	542.10	326.62	349.69	-130.149 *	139.206 *	-8.079

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^\circ - H_0^\circ$	kJ	MOLAR VOLUME	9.9300 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES			99.300 cm ³

SiO₂..... ALPHA - BETA TRANSITION 844 K.

H₂O..... B. P. 372.8 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 908.360 - 0.105663 T - 1.11953 \times 10^{-4} T^{-0.5} + 3.80445 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 900 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

63

Halloysite

FORMULA WEIGHT 258.161

Al₂Si₂O₅(OH)₄: Crystals 298.15 to 900 K.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H _T ^o -H ₂₉₈ ^o)/T	S _T ^o	-(G _T ^o -H ₂₉₈ ^o)/T	C _P ^o	ENTHALPY	FREE ENERGY	LOG K
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	203.33	203.33	245.25	-4101.028	-3780.372	662.308
UNCERTAINTY		3.07	3.07	0.76	(1.200)	(1.508)	(0.264)
400	68.590	282.17	213.58	289.86	-4102.532	-3670.485	479.318
500	115.774	350.01	234.24	317.06	-4101.529	-3562.569	372.181
600	150.860	409.45	258.59	334.19	-4099.244	-3454.963	300.783
700	177.866	461.83	283.96	344.69	-4096.431	-3347.815	249.818
800	199.125	508.28	309.16	350.55	-4093.619	-3241.057	211.620
900	216.116	549.74	333.63	353.05	-4091.187	-3134.609	181.929

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	J/bar

TRANSITIONS IN REFERENCE STATE ELEMENTS

ALUMINUM... M. P. 933 K.

SILICON... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 772.300 - 7.25884 \times 10^{-2} T - 8.72948 \times 10^{-3} T^{-0.5} + 1.93671 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 900 K)

COMPILED 9-30-79

64 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Halloysite

FORMULA WEIGHT 258.161

$Al_2Si_2O_5(OH)_4$: Crystals 298.15 to 900 K.

TEMP. K	$(H_T^\circ - H_{298}^\circ)/T$ J/mol·K	S_T° J/mol·K	$-(G_T^\circ - H_{298}^\circ)/T$ J/mol·K	C_P° J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	203.33	203.33	245.25	-32.303 *	-11.332 *	1.985
UNCERTAINTY		3.07	3.07	0.76	1.200	1.508	0.264
400	68.590	282.17	213.58	289.86	-118.715 *	2.820 *	-0.368
500	115.774	350.01	234.24	317.06	-116.572 *	32.958 *	-3.443
600	150.860	409.45	258.59	334.19	-114.416 *	62.663 *	-5.455
700	177.866	461.83	283.96	344.69	-112.669 *	92.036 *	-6.868
800	199.125	508.28	309.16	350.55	-111.643 *	121.190 *	-7.913
900	216.116	549.74	333.63	353.05	-112.134 *	150.344 *	-8.726

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

TRANSITIONS IN REFERENCE STATE OXIDES

SiO_2 ALPHA - BETA TRANSITION 844 K.

H_2O B. P. 372.8 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 772.300 - 7.25884 \times 10^{-2} T - 8.72948 \times 10^{-3} T^{-0.5} + 1.93671 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 900 K)

COMPILED 9-30-79

Pyrophyllite

FORMULA WEIGHT 360.316

$Al_2Si_4O_{10}(OH)_2$: Crystals 298.15 to 1200 K.

TEMP. K	$(H_T^\circ - H_{298}^\circ)/T$ J/mol·K	S_T° J/mol·K	$-(G_T^\circ - H_{298}^\circ)/T$ J/mol·K	C_P° J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	239.42	239.42	294.35	-5642.023 (1.158)	-5268.128 (1.043)	922.958 (0.183)
UNCERTAINTY		0.99	0.99	0.32			
400	82.857	334.64	251.78	351.98	-5643.701	-5140.001	671.218
500	140.574	417.37	276.79	388.51	-5642.249	-5014.219	523.834
600	184.173	490.62	306.45	414.70	-5638.987	-4888.874	425.616
700	218.683	556.21	337.53	436.37	-5634.491	-4764.208	355.511
800	247.188	615.83	368.64	457.14	-5628.927	-4640.239	302.978
900	271.728	670.93	399.20	479.33	-5622.197	-4517.011	262.162
1000	293.717	722.70	428.99	504.51	-5635.343	-4393.128	229.474
1100	314.175	772.12	457.95	533.75	-5624.573	-4269.422	202.739
1200	333.858	819.99	486.13	567.86	-5611.069	-4146.752	180.504

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
$H_{298}^\circ - H_0^\circ$	42.695 kJ	MOLAR VOLUME	12.5900 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS			125.900 cm ³

ALUMINUM... M. P. 933 K.

SILICON... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^\circ = 1454.51 - 0.396093 T + 3.97189 \times 10^{-4} T^2 - 1.77428 \times 10^{-4} T^{-0.5} + 6.06936 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 200 - 1200 K)

COMPILED 09-30-79

66 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Pyrophyllite

FORMULA WEIGHT 360.316

Al₂Si₄O₁₀(OH)₂: Crystals 298.15 to 1200 K.

TEMP. K					FORMATION FROM THE OXIDES GIBBS		
	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	239.42	239.42	294.35	-37.708 *	-23.623 *	4.139
UNCERTAINTY		0.99	0.99	0.32	1.158	1.043	0.183
400	82.857	334.64	251.78	351.98	-81.004 *	-15.294 *	1.997
500	140.574	417.37	276.79	388.51	-79.982 *	1.014 *	-0.106
600	184.173	490.62	306.45	414.70	-79.092 *	17.128 *	-1.491
700	218.683	556.21	337.53	436.37	-78.475 *	33.117 *	-2.471
800	247.188	615.83	368.64	457.14	-78.024 *	49.019 *	-3.201
900	271.728	670.93	399.20	479.33	-78.611 *	65.009 *	-3.773
1000	293.717	722.70	428.99	504.51	-73.322 *	80.701 *	-4.215
1100	314.175	772.12	457.95	533.75	-66.033 *	95.770 *	-4.548
1200	333.858	819.99	486.13	567.86	-56.262 *	110.073 *	-4.791

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING		ENTHALPY OF VAPORIZATION	
H ₂₉₈ ^o - H ₀ ^o	42.695 kJ	MOLAR VOLUME	12.5900 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES			125.900 cm ³

SiO₂..... ALPHA - BETA TRANSITION 844 K.

H₂O..... B. P. 372.8 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 1454.51 - 0.396093 T + 3.97189 \times 10^{-4} T^2 - 1.77428 \times 10^{-6} T^{-0.5} + 6.06936 \times 10^6 T^{-2}$$

(EQUATION VALID FROM 200 - 1200 K)

COMPILED 09-30-79

Margarite

FORMULA WEIGHT 398.187

CaAl₄Si₂O₁₀(OH)₂: Crystals 298.15 to 1200 Y.

TEMP. K	FORMATION FROM THE ELEMENTS GIBBS						
	(H _T ^o -H ₂₉₈ ^o)/T	S _T ^o	-(C _T ^o -H ₂₉₈ ^o)/T	C _P ^o	ENTHALPY	FREE ENERGY	LOG K
	J/mol·K	J/mol·K	J/mol·K	J/mol·K	kJ/mol	kJ/mol	
298.15	0.000	263.64	263.64	323.44	-6239.610	-5854.840	1025.748
UNCERTAINTY		0.66	0.66	0.38	(1.954)	(1.906)	(0.334)
400	90.817	368.01	277.20	385.02	-6241.515	-5722.938	747.342
500	153.852	458.44	304.59	424.47	-6239.969	-5593.442	584.345
600	201.397	538.43	337.03	452.28	-6236.538	-5464.421	475.722
700	238.771	609.76	370.99	472.77	-6232.139	-5336.092	398.186
800	269.036	673.95	404.92	488.32	-6228.124	-5208.304	340.069
900	294.096	732.19	438.10	500.33	-6223.379	-5081.086	294.900
1000	315.207	785.41	470.21	509.71	-6261.818	-4951.351	258.633
1100	333.238	834.35	501.12	517.09	-6256.875	-4820.543	228.909
1200	348.810	879.60	530.79	522.88	-6259.005	-4689.547	204.132

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	13.3800 J/bar 133.800 cm ³

TRANSITIONS IN REFERENCE STATE ELEMENTS

CALCIUM... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

ALUMINUM... M. P. 933 K.

SILICON... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 826.504 - 2.51455 \times 10^{-2} T + 8.42744 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1200 K)

COMPILED 9-30-79

68 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Margarite

FORMULA WEIGHT 398.187

CaAl₄Si₂O₁₀(OH)₂: Crystals 298.15 to 1200 K.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	263.64	263.64	323.44	-145.888 *	-137.205 *	24.038
UNCERTAINTY		0.66	0.66	0.38	1.954	1.906	0.334
400	90.817	368.01	277.20	385.02	-189.496 *	-130.674 *	17.064
500	153.852	458.44	304.59	424.47	-188.597 *	-116.067 *	12.125
600	201.397	538.43	337.03	452.28	-187.465 *	-101.661 *	8.850
700	238.771	609.76	370.99	472.77	-186.305 *	-87.450 *	6.526
800	269.036	673.95	404.92	488.32	-185.271 *	-73.407 *	4.793
900	294.096	732.19	438.10	500.33	-185.056 *	-59.405 *	3.448
1000	315.207	785.41	470.21	509.71	-182.503 *	-45.579 *	2.381
1100	333.238	834.35	501.12	517.09	-179.874 *	-32.013 *	1.520
1200	348.810	879.60	530.79	522.88	-177.274 *	-18.684 *	0.813

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	13.3800 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES			133.800 cm ³

SiO₂..... ALPHA - BETA TRANSITION 844 K.

H₂O..... B. P. 372.8 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 826.504 - 2.51455 \times 10^{-2} T - 8.42744 \times 10^{-3} T^{-0.5}$$

(EQUATION VALID FROM 200 - 1200 K)

COMPILED 9-30-79

PROPERTIES AT HIGH TEMPERATURES

69

Prehnite

FORMULA WEIGHT 412.390

Ca₂Al₂Si₃O₁₀(OH)₂: Crystals 298.15 to 1200 K.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE ELEMENTS GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	292.74	292.74	331.11	-6193.631	-5816.426	1019.018
UNCERTAINTY		0.72	0.72	0.44	(1.699)	(1.643)	(0.288)
400	92.227	398.77	306.54	389.19	-6194.649	-5687.254	742.682
500	155.666	489.97	334.30	427.23	-6192.499	-5560.630	580.918
600	203.247	570.33	367.08	453.51	-6188.659	-5434.572	473.124
700	240.393	641.71	401.31	471.95	-6184.068	-5309.269	396.184
800	270.195	705.62	435.43	484.90	-6180.839	-5184.434	338.510
900	294.580	763.29	468.71	493.85	-6176.300	-5060.122	293.683
1000	314.825	815.65	500.82	499.76	-6194.040	-4934.788	257.768
1100	331.815	863.46	531.65	503.32	-6190.898	-4809.038	228.363
1200	346.188	907.34	561.15	505.00	-6202.613	-4682.244	203.814

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	14.0330 J/bar
TRANSITIONS IN REFERENCE STATE ELEMENTS			140.330 cm ³

CALCIUM... ALPHA-BETA 737, M. P. BETA 1123, B. P. 1755 K.

ALUMINUM... M. P. 933 K.

SILICON... M. P. 1685 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 946.022 - 5.75327 \times 10^{-2} T - 1.05605 \times 10^{-4} T^{-0.5} + 2.75523 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 1200 K)

COMPILED 9-30-79

70 THERMODYNAMIC PROPERTIES OF SELECTED MINERALS

Prehnite

FORMULA WEIGHT 412.390

Ca₂Al₂Si₃O₁₀(OH)₂: Crystals 298.15 to 1200 K.

TEMP. K	(H _T ^o -H ₂₉₈ ^o)/T J/mol·K	S _T ^o J/mol·K	-(G _T ^o -H ₂₉₈ ^o)/T J/mol·K	C _P ^o J/mol·K	FORMATION FROM THE OXIDES GIBBS		
					ENTHALPY kJ/mol	FREE ENERGY kJ/mol	LOG K
298.15	0.000	292.74	292.74	331.11	-229.827 *	-221.281 *	38.768
UNCERTAINTY		0.72	0.72	0.44	1.699	1.643	0.288
400	92.227	398.77	306.54	389.19	-273.427 *	-214.797 *	28.050
500	155.666	489.97	334.30	427.23	-272.506 *	-200.243 *	20.919
600	203.247	570.33	367.08	453.51	-271.442 *	-185.887 *	16.183
700	240.393	641.71	401.31	471.95	-270.585 *	-171.696 *	12.812
800	270.195	705.62	435.43	484.90	-270.210 *	-157.608 *	10.291
900	294.580	763.29	468.71	493.85	-271.398 *	-143.419 *	8.324
1000	314.825	815.65	500.82	499.76	-269.431 *	-129.301 *	6.754
1100	331.815	863.46	531.65	503.32	-267.725 *	-115.376 *	5.479
1200	346.188	907.34	561.15	505.00	-266.440 *	-101.583 *	4.422

MELTING POINT	K	BOILING POINT	K
ENTHALPY OF MELTING	kJ	ENTHALPY OF VAPORIZATION	kJ
H ₂₉₈ ^o - H ₀ ^o	kJ	MOLAR VOLUME	14.0330 J/bar
TRANSITIONS IN REFERENCE STATE OXIDES			140.330 cm ³

SiO₂..... ALPHA - BETA TRANSITION 844 K.

H₂O..... B. P. 372.8 K.

HEAT CAPACITY EQUATION(S)

$$C_P^o = 946.022 - 5.75327 \times 10^{-2} T - 1.05605 \times 10^{-4} T^{-0.5} + 2.75523 \times 10^{-6} T^{-2}$$

(EQUATION VALID FROM 200 - 1200 K)

COMPILED 9-30-79

