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THERMODYNAMIC AND THERMOPHYSICAL PROPERTIES OF SELECTED PHASES IN THE $MgO-SiO_2-H_2O-CO_2$, $CaO-Al_2O_3-SiO_2-H_2O-CO_2$, AND $Fe-FeO-Fe_2O_3-SiO_2$ CHEMICAL SYSTEMS, WITH SPECIAL EMPHASIS ON THE PROPERTIES OF BASALTS AND THEIR MINERAL COMPONENTS

By

Gilpin R. Robinson, Jr., John L. Haas, Jr.,
Constance M. Schafer, and H.T. Haselton, Jr.

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AUTHOR(S): Gilpin R. Robinson, Jr., John L. Hass, Jr., Constance M. Schafer, and H. T. Haselton, Jr.

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Contents

List of tables

List of figures

Thermodynamic and Thermophysical Properties of Selected Phases in the $MgO-SiO_2-H_2O-CO_2$, $CaO-Al_2O_3-SiO_2-H_2O-CO_2$, and $Fe-FeO-Fe_2O_3-SiO_2$ Chemical Systems, with Special Emphasis on the Properties of Basalts and Their Mineral Components

Gilpin R. Robinson, Jr., and John L. Haas, Jr.
Constance M. Schafer and H. T. Haselton, Jr.

National Center for the Thermodynamic Data of Minerals,

U.S. Geological Survey, Reston, VA 22091

1.1. Introduction

The thermal and chemical environment of a potential nuclear waste repository must be known and understood before an intelligent decision can be made regarding radioactive waste storage. A properly evaluated set of thermodynamic data can provide some of the needed information. This report contains a tabulation of thermodynamic and thermophysical properties for selected phases in the $MgO-SiO_2-H_2O-CO_2$, $Fe-FeO-Fe_2O_3-SiO_2$, and $CaO-Al_2O_3-SiO_2-H_2O-CO_2$ chemical systems and presents the procedure used to evaluate the internally consistent set of thermodynamic data for minerals.

The chapter is divided into five sections. The first section is a brief introduction. The second section summarizes the chemical and physical character of basalt rock and identifies:

1. a generalized chemical system describing the rock type,
2. major mineral constituents,
3. minor mineral constituents, and
4. common alteration phases.

The third section describes the procedure used to evaluate the inter-

nally consistent set of thermodynamic and thermophysical properties for mineral phases presented as tables in the Appendix. A procedure to estimate thermophysical properties of minerals and rocks is described. Section 4 contains reference citations to the sources of data used in the evaluation, and section 5 (Appendix) contains tables of thermodynamic and thermophysical properties for selected phases and critiques the specific sources of information used in the evaluation of these properties.

1.2. Physical, Chemical, and Mineralogical Characteristics of Flood Basalt

1.2.1. Introduction

Flood basalt occurs as sheets of rapidly cooled basaltic lava erupted from a volcanic center in continental basement. Individual sheets typically have great areal extent and range between less than 1 meter to 100 meters in thickness.

The model chemical system is CaO-(Na_2O)-FeO-(Fe_2O_3)-MgO-Al_2O_3-SiO_2-(H_2O,CO_2). Oxide components in parenthesis are of lesser importance. A typical analysis, norm, and mode is given in table 1.

The mineral constituents of basalts and altered basalts are given below with their chemical formulas. Many mineral phases have variable composition and can be described as a solid solution of end-member phases having different chemical compositions but identical crystal structures. Mineral phases commonly showing variable composition are listed under their general name (for example, olivine), followed by the names and formulas of the important end-member phases of the solid solution series (for example, Forsterite (For), Fayalite (Fay)). Where appropriate, typical compositions of the phases showing variable composition are given in mole percent of the end-member phases (for example, olivine - typically For 84:Fay 16). Mineral phases (for example, zeolites), classed in groups having similar properties and similar, but not identical, crystal structures, are listed in a similar manner.

Table 1. Representative flood basalt composition, norm, and mode

Oxide wt. %	Basalt[a]	Norm (wt. %) (calculated from chemical composition)	
Chemical composition		Quartz	3.9
SiO_2	53.8	K-feldspar	8.9
TiO_2	2.0	Albite	25.2
Al_2O_3	13.9	Anorthite	20.0
Fe_2O_3	2.6	Diopside	13.9
FeO	9.3	Hypersthene	15.3
MnO	0.2	Ilmenite	3.8
MgO	4.1	Magnetite	3.7
CaO	7.9	Apatite	0.9
Na_2O	3.0	TOTAL	98.6
K_2O	1.5		
H_2O	1.2	Mode (measured) (volume %)	
P_2O_5	0.4	Plagioclase	<1
TOTAL	99.9	Orthopyroxene	<5
		Clinopyroxene	<5
		Olivine	<5
		Matrix	>90[b]
		An content of Plagioclase (mole %)	63
		TOTAL	100.0

[a]Average Yakima basalt (analysis b, p. 593), Columbia River Plateau, Washington-Oregon, Waters, 1961.

[b]Matrix comprises: intergrown microcrystalline clinopyroxene (pigeonite), orthopyroxene, and plagioclase with minor cristobalite (listed in order of decreasing abundance).

1.2.2. Major Constituents

The major constituents consist of phenocrysts and matrix phases. Phenocrysts typically account for 0 to 10 percent of the rock volume with matrix comprising the remainder. Gas bubbles (vesicles) occur in some basalt units, usually near the top surface of the flow.

1. Phenocrysts usually are:

Olivine	-	typically For 84:Fay 16
Forsterite (For)	-	Mg_2SiO_4
Fayalite (Fay)	-	Fe_2SiO_4
Plagioclase	-	typically Ano 60:Alb 40
Anorthite (Ano)	-	$CaAl_2Si_2O_8$
Albite (Alb)	-	$NaAlSi_3O_8$

2. Matrix, which typically is a microcrystalline intergrowth of:

Clinopyroxene	-	typically pigeonite - approximately Cen 46:Cfs 38:Dio 9:Hed 7
Diopside (Dio)	-	$CaMg(SiO_3)_2$
Hedenbergite (Hed)	-	$CaFe(SiO_3)_2$
Clinoenstatite (Cen)	-	$MgSiO_3$
Clinoferrosilite (Cfs)	-	$FeSiO_3$
Hypersthene	-	approximately Ens 60:Fes 40
Enstatite (Ens)	-	$MgSiO_3$
Ferrosilite (Fes)	-	$FeSiO_3$
Plagioclase		
Anorthite (Ano)	-	$CaAl_2Si_2O_8$
Albite (Alb)	-	$NaAlSi_3O_8$

1.2.3. Alteration Products

Alteration products typically occur in vesicles or along fractures and flow-unit contacts in basalts. The low- and intermediate-temperature alterations are temperature-induced responses to fluids (whether heated or not) moving through the rock, and most of the alteration phases require the addition of either water or carbon dioxide to the rock. The intermediate- and high-temperature alterations are a result of thermal metamorphism of the rock body. Basalts which have experienced thermal metamorphism may show pervasive alteration.

1. Low temperature ($T < 250°C$) reactions typically produce the following minerals:

Calcite (Cal) - $CaCO_3$

Dolomite (Dol) - $CaMg(CO_3)_2$

Epidote (Epi) - Zoisite (Zoi) - $Ca_2FeAl_2Si_3O_{12}(OH) - Ca_2Al_3Si_3O_{12}(OH)$

Prehnite (Pre) - $Ca_2Al_2Si_3O_{10}(OH)_2$

Lawsonite (Law) - $CaAl_2Si_2O_7(OH)_2 \cdot H_2O$

Zeolites

- Laumontite (Lau) - $CaAl_2Si_4O_{12} \cdot H_2O$
- Heulandite (Heu) - $CaAl_2Si_7O_{18} \cdot 6H_2O$
- Analcite (Ana) - $NaAlSi_2O_6 \cdot H_2O$
- Wairakite (Wai) - $CaAl_2Si_4O_{12} \cdot 2H_2O$

2. Intermediate temperature ($T < 375°C$) reactions typically produce the following minerals:

Calcite (Cal) - $CaCO_3$

Dolomite (Dol) - $CaMg(CO_3)_2$

Albite (Alb) - $NaAlSi_3O_8$

Zoisite (Zoi) - $Ca_2Al_3Si_3O_{12}(OH)$

Chlorite (Clinochlore) (Cln) - $Mg_5Al_2Si_3O_{10}(OH)_4$

Amphibole

Tremolite (Tre) - $Ca_2Mg_5Si_8O_{22}(OH)_2$

Actinolite (Act) - $Ca_2Fe_5Si_8O_{22}(OH)_2$

Anthophyllite (Ant) - $Mg_7Si_8O_{22}(OH)_2$

3. High temperature ($T > 350°C$) reactions typically produce the following minerals:

Amphibole - commonly Hornblende - $Na_xCa_2(Mg,Fe)_{5-2y}Al_{x+4y}Si_{8-x-2y}O_{22}(OH)_2$

$x \approx 0\text{-}1$, $y \approx 0.5$

Garnet - typically Almandine or Grossular

Grossular (Gro) - $Ca_3Al_2Si_3O_{12}$

Almandine (Alm) - $Fe_3Al_2Si_3O_{12}$

Pyrope (Pyr) - $Mg_3Al_2Si_3O_{12}$

Clinopyroxene

Hedenbergite (Hed) - $CaFe(SiO_3)_2$

Diopside (Dio) - $CaMg(SiO_3)_2$

Ca-Al Clinopyroxene (Cat) - $CaAl_2SiO_6$

Wollastonite (Wol) - $CaSiO_3$

Othopyroxene

Enstatite (Ens) - $MgSiO_3$

Ferrosilite (Fes) - $FeSiO_3$

Olivine

Forsterite (For) - Mg_2SiO_4

Fayalite (Fay) - Fe_2SiO_4

Spinel

Magnetite (Mgt) - Fe_3O_4

Hercynite (Her) - $FeAl_2O_4$

1.3. Thermodynamic and Thermophysical Properties

1.3.1. Introduction

1.3.1.1. Definitions and notation

Heat capacity is defined as the quantity of heat required to raise the temperature of a unit quantity of a substance one degree kelvin at constant pressure. The heat capacity is generally normalized per unit mass or per unit volume of the substance. "Specific heat" is defined as the heat capacity per gram of the substance. "Molar heat capacity" is defined as the heat capacity per gram formula weight of the substance. "Thermal capacity" is defined as the heat capacity per unit volume of the substance.

Thermodynamic properties of an extensive nature, such as volume, heat capacity, entropy, enthalpy, and Gibbs energy, will be presented in units normalized per molar quantity of each phase. This choice is convenient since the thermodynamic properties describing reactions among minerals are easily expressed and calculated in "molar" units. "Specific heat" will be used to describe the thermal properties of rocks and mineral aggregates.

Relative enthalpy is defined as the quantity of heat required to change the temperature of a unit quantity of substance from a reference temperature (T_r) to another temperature (T). Relative enthalpy is related to heat capacity by the following thermodynamic identity.

$$H_T - H_{T_r} = \int_{T_r}^{T} C_p \, dT \qquad (1)$$

Calorimetric entropy is defined as

$$S_T - S_0 = \int_0^T \frac{C_p}{T} dT \qquad (2)$$

and is determined from experimental low-temperature heat-capacity data.

Thermodynamic entropy, S_T, is defined as the sum of calorimetric entropy and residual or zero-point entropy, S_0. Non-zero values for residual entropy can arise from configurational entropies related either to disorder among crystallographic sites or molecular disorder, or to the lack of significant magnetic ordering at those temperatures reached by the heat capacity measurements.

Molar volume, V, is defined as the volume occupied by one mole of a phase and is a function of pressure and temperature. Enthalpy, as a function of temperature and pressure, is related to heat capacity and molar volume by the thermodynamic identity

$$H_{T,P} = H_0 + \int_0^T C_p \, dT + \int_{P_r}^P (V_T - T(\frac{\partial V}{\partial T})_P) \, dP \qquad (3)$$

where H_0 is the zero-point contribution to enthalpy at the reference state pressure. Entropy, as a function of pressure is related to molar volume by the thermodynamic identity

$$S_{T,P} = S_{T,P_r} - \int_{P_r}^P (\frac{\partial V}{\partial T})_P \, dP. \qquad (4)$$

Gibbs energy is related to enthalpy and entropy by the thermodynamic identity

$$G_{T,P} = H_{T,P} - T\,S_{T,P}. \quad (5)$$

The isobaric coefficient of thermal expansion, α_P, and the isothermal coefficient of compressibility, β_T, are related to molar volume by the following identities

$$\alpha_P = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P \quad (6)$$

$$\beta_T = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T. \quad (7)$$

1.3.1.2. Types of data used in study

Data from three general categories of experimental techniques have been used in the evaluation of the heat capacity, relative enthalpy, and calorimetric entropy. Data from low-temperature calorimetry was used in the evaluation to supply accurate values of heat capacity, at temperatures generally 200-300 K, and calorimetric entropy at 298 K. Data from differential scanning calorimetry was used to supply values of heat capacity at temperatures 300-800 K. Data from drop calorimetry was used to evaluate mineral heat capacities and relative enthalpies at temperatures generally 300-1800 K.

Volume as a function of temperature and pressure may be measured directly, as in x-ray crystallography, or determined as a change in volume under changing pressure and temperature conditions from a reference state (relative volume measurements).

Data from enthalpy-of-reaction measurements, including solution calorimetry and combustion calorimetry, measure the enthalpy of a phase relative to other phases.

Data from phase-equilibrium experiments and EMF measurements supply measurements of the Gibbs energy of a phase relative to other phases.

The simultaneous evaluation procedure followed in this study and the relationships among thermodynamic properties shown in equations 1 to 7 allow the direct measurement of individual thermodynamic properties to supply indirect constraints on the permissible values of the other thermodynamic properties.

1.3.1.2.1. Low-temperature calorimetry

Low-temperature calorimetry is used to obtain accurate heat capacities and calorimetric entropies for substances at temperatures generally below 300 K. McCullough and Scott (1968, Ch. 4-5) provide an excellent description of the design and operation of low-temperature calorimeters. The heat capacity of an unknown sample is determined by accurately measuring the heat energy (electrical) added to a sample in a calorimeter to change its temperature by a measured amount. The calorimeter is cooled to its initial low temperature by a liquified gas. The calorimeter is shielded to minimize heat exchange between the calorimeter and its surroundings. The heat capacity of the sample is determined at closely spaced temperature intervals, using the formula:

$$\frac{dE}{dt} - \left(\frac{dE}{dT}\right)_{cal} \frac{dT}{dt} = MC_p \frac{dT}{dt}$$

where E is heat energy

$\left(\frac{dE}{dT}\right)_{cal}$ is the heat effect of the calorimeter as temperature is changed

t is time

T is temperature (kelvin)

M is mass of sample/molar weight of sample

C_p is heat capacity of sample

The temperature range of operation is generally between 5 and 300 K, with a precision better than 0.1 percent for heat capacity. The calorimetric entropy (S_T-S_0) is determined using the formula:

$$S_T - S_0 = \int_0^T C_p/T \, dT.$$

The precision of measurement is generally better than 0.2 percent.

Data from low-temperature calorimetry was used to constrain the evaluation for entropy and for heat capacity of structural components above 200 K.

1.3.1.2.2 Differential Scanning Calorimetry

McNaughton and Mortimer (1975) provide an excellent description of the operation and use of a differential scanning calorimeter to measure heat capacity. Differential Scanning Calorimetry (DSC) is used to determine the heat capacity of a substance by measuring the differential heat flow required to maintain the sample and an inert reference material at the same temperature, when both are heated. The sample and reference are subjected to a programmed linear temperature change, and the rates of heat flow into the sample and reference are proportional to their instantaneous specific heat. Heat capacity as

a function of temperature can be obtained by evaluating the differential rate of heat flow between the sample and reference, as a function of temperature, using the formula:

$$C_p(s) = \frac{M(r)}{M(s)} \frac{(dT/dt)(r)}{(dT/dt)(s)} \frac{(dE/dt)(s)}{(dE/dt)(r)}$$

where E is heat energy

t is time

T is temperature (kelvin)

M is mass of sample/mol wt. of sample

C_p is molar heat capacity of the respective materials

Subscript s refers to sample material

Subscript r refers to reference material.

The heat capacity of the reference material is known.

The temperature range of operation is generally between 300 and 800 K (27-527°C), with a precision of measurement estimated to be better than 1.0 percent and often as low as 0.3%.

1.3.1.2.3. Drop calorimetry

The enthalpy change of a substance is determined by measuring the heat flow from a sample as it is dropped from a known temperature into a calorimeter held at a constant reference temperature. McCullough and Scott (1968, Ch. 8) provide an excellent description of drop calorimetry. The heat capacity of the sample can be determined from a series of drop calorimetry measurements with differing initial temperatures by evaluating the differential enthalpy changes as a function of temperature using the formula:

$$\frac{d(H_T - H_{T_r})}{dT} = MC_p$$

where $H_T - H_{T_r}$ is the measured enthalpy change between the sample at the initial temperature and reference temperature, corrected for the heat effects of the sample container

T is temperature (kelvin)

M is mass of sample/molecular weight of sample

C_p is molar heat capacity of sample

The temperature range of operation is generally between 273 and 1600 K (0 to 1327°C), with a precision of measurement, on modern equipment, estimated to be 0.2 percent. The precision of measurement from older literature sources is estimated to be approximately 0.5 percent.

1.3.1.2.4. X-ray crystallography

The measurement of molar volume by x-ray crystallography is based upon the determination of crystallographic lattice dimensions from the diffraction of a collimated beam of monochromatic x-rays that is scattered by atoms in the crystal lattice. A general description of measurement techniques is provided by Krishnan and others (1979) and Hazen (1976a). Volume measurements at temperatures above room temperature are generally produced using a heating mechanism and a calibrated thermocouple to measure sample temperature. The temperature range of measurement is generally between 297 and 1400 K (24-1127°C) depending upon the stability of the sample and equipment design. Volume measurement at pressures greater than 1 atmosphere are generally produced

using a minature diamond pressure cell (Merrill and Bassett, 1975). Pressures are generated by squeezing the sample and an internal standard between two diamond plates, and sample pressures are determined by measuring the lattice parameters of the internal standard whose volume properties as a function of pressure are known. The pressure range of measurement is generally between 10,000 and 100,000 bars, depending, again on sample stability and equipment design. The measurement of lattice dimensions using the x-ray technique has a precision of measurement generally between 0.02 and 0.5 percent of the measured value, and typically is approximately 0.1 percent of the observed value. The precision of temperature determination is generally better than ± 10°C, and the precision of pressure measurement is generally between ± 1000 and 2000 bars.

1.3.1.2.5. Relative-volume measurements

The measurement of molar volume by relative-volume techniques is based upon the determination of a change in volume or linear dimensions of a sample and container as pressure or temperature is changed from reference conditions. A general description of techniques for relative-volume measurements as a function of temperature is given by Krishnan and others (1979). The sample is heated from a reference temperature to a measurement temperature, and sample temperature is generally determined from a calibrated thermocouple attached to the sample. The volume change is determined by accurately measuring the change in linear dimensions of the sample. The change in linear dimensions can frequently be measured with a precision better than 1 percent (depending upon calibration and equipment design), with a precision of

temperature measurement better than ± 10°C. The range of measurement is generally between 298 and 1400 K (24-1127°C).

A general description of techniques to measure relative volume as a function of pressure is given by Vaidya and Kennedy (1970). The sample is packed in a container and placed in a pressure bomb of known volume filled with a hydrostatic pressure medium (a fluid or solid with low-yield strength). Pressure is increased from a reference pressure by displacement of a piston into the pressure bomb chamber, and pressures are measured by gauge. The volume change is determined from the displacement of the piston after correcting for the volume compressibility of the pressure medium and sample container. The range of measurement is generally between 1000 bars and 50,000 bars, with a precision of pressure measurement generally between 100 and 1000 bars. The precision of relative volume measurement is approximately 1 percent.

1.3.1.2.6. Enthalpy-of-reaction measurements

The enthalpy of reaction between phases is determined by measuring the heat effects of a reaction or a step-wise series of reactions in a calorimeter of similar design to those described in sections 1.3.1.2.1 and 1.3.1.2.3. Combustion calorimetry directly measures the enthalpy of reaction between a known quantity of a phase (usually an element), gas, and the product phases after sustained combustion. Solution calorimetry indirectly measures the enthalpy of reaction among phases by measuring the heat effects of dissolution of a known quantity of "product" phases of the reaction in a solvent versus the heat effects

of dissolution of a known quantity of "reactant phases" in the solvent. Since the solution formed from the dissolution of product and reactant phases are identical, the enthalpy of reaction between reactant and product phases is equal to the difference of the heat effects of the dissolution reactions.

Low-temperature (generally between 298 and 370 K) solution calorimetry generally utilizes HF as the solvent for silicate minerals. Problems with use are the slow dissolution rates of some phases and the non-equilibrium precipitation of fluoride phases during the dissolution process. High-temperature (generally between 900 and 1100 K) solution calorimetry generally utilizes molten salts (often borates) as the solvent. An advantage of high-temperature calorimetry is that reaction rates are generally fast. One limitation is that phases containing volatile components or phases stable only at low temperatures at one atmosphere cannot be studied.

In borate-melt solution calorimetry, the volume ratio of solvent to reactant phase is very large. Since the solvent melts remain essentially "isochemical" during the dissolution process, it has been assumed that the heat of mixing effects between the "reactant" components in the solvent will be negligably small. This simplifies the determination of the enthalpy of reaction among phases since the enthalpy of reaction can be computed from the sum of the heat effects of dissolution of each of the reactant phases in pure solvent minus the sum of the heat effects of dissolution of each of the product phases.

The precision of measurement of both low- and high-temperature calorimetry varies between 0.3 and 2 percent of the observed value, depending upon the kinetics of the dissolution process and equipment design.

1.3.1.2.7. Phase equilibria experiments

Phase equilibria experiments measure the Gibbs energy of a phase by reference to the Gibbs energy of other phases, which together define a reaction monitored by experiment. Edgar (1973) and Ulmer (1971) provide descriptions of equipment and techniques used in phase equilibria experiments. Two types of experiments are typically performed to measure phase equilibria.

1. In the reaction-reversal technique, pressure, temperature, and the direction of a univarient reaction is measured. By determining two closely spaced pressure-temperature points between which the reaction reverses direction, a narrow interval bracketing a point where the free energy of reaction among the assembled phases is zero has been determined. The direction of reaction is frequently determined by starting the experiment with a mixture of product and reactant phases and using some technique on the result of the experiment to determine the increase or decrease in abundance of each of the assembled phases (often x-ray analysis, or weight loss-gain studies of individual phases). If x-ray analysis is used, the minimum amount of change in abundance of a phase that can be measured is approximately five percent, by volume.

2. In the activity-measurement technique, pressure, temperature, and the composition (activity) of a phase (or phases) of variable composition is measured in a divariant assemblage of phases. If the composition-activity relationship is known for the phase of variable composition, and the assemblage of phases has reached equilibrium, then the free energy of reaction among an idealized assemblage of phases of fixed

composition can be calculated for the measured pressure and temperature conditions. Examples of this technique are the silicic acid experiments of Hemley and others (1977a, 1977b, 1980), the vapor pressure measurements of H_2O equilibrated with periclase and brucite (Kennedy, 1956; Fyfe, 1958; Barnes and Ernst, 1963), and the vapor pressure measurements of CO_2 equilibrated with periclase and magnesite (Marc and Simek, 1913). An essential feature of this technique is the demonstration that equilibrium among phases has been achieved during the experiment. This can be done by setting up duplicate experiments at a pressure-temperature condition using initial compositions of the variable phase which bracket the equilibrium composition (eg. Hemley and others, 1977b). Equilibrium among phases can be inferred from experiments which monitor the composition of the variable phase as a function of time. At times greater than the time in which no or little change can be observed in the composition of the variable phase, equilibrium can be presumed. It should be noted that this criteria, by itself, does not demonstrate "equilibrium", but only indicates that the rate of approach to "equilibrium" is too slow to be measured by experiment.

The precision of measurement in phase-equilibrium experiments is controlled by the dilligence of the experimentalist, kinetics of reactions, and measurement uncertainties of temperature, pressure, phase composition, and abundance of phases. The precision of measurement of temperature and pressure is approximately ± 1 to 10°C, and ± 100 to 500 bars for pressures less than 8000 bars, and ± 500 to 1000 bars for pressures greater than 8000 bars. The precision of measurement of composition or change in abundance of phases depends upon the design of the equipment, but typically is a few percent of the variable measured.

The temperature-pressure window bracketing a reaction reversal is commonly measured with a precision of ± 5-20°C and ± 100-1000 bars.

1.3.1.2.8. Electromotive-force measurements

In electromotive force (EMF) measurements, the Gibbs energy of a reaction is determined by measuring the electrochemical potential for ion migration through an electrolyte (which is an impervious barrier to everything else) separating assemblages of phases which are either 1) unstable with respect to each other, or 2) both define an activity of the mobile ion. The book, Electromotive Force Measurements in High-Temperature Systems (Alcock (ed.), 1968), supplies a description of equipment and techniques frequently used in the measurement of EMF.

A high impedence potentiometer is used to measure the potential energy. The electromotive potential is related to free energy by the relationship

$$E = -\frac{1}{n\mathcal{F}} \sum_{i=1}^{j} N_i G_i$$

where N_i is the stoichiometric coefficient for the ith phase and is positive for products and negative for reactants.

G_i is the Gibbs energy of the ith phase,

E is electrochemical potential, in volts,

$\mathcal{F}$ is the Faraday constant,

j is the number of phases in the reaction, and

n is the number of electrons transferred during the reaction.

The precision of measurement of electrochemical potential is generally ± 1 millivolt but, under special conditions, can be as small as ± 0.1 millivolt. The precision of measurement is related to the kinetics of the reaction, with kinetically fast reactions having better precision. Failure to accurately determine free energy of reaction from EMF measurements usually results from the following problems:

1. electrical conductivity of the electrolyte (varies with temperature and electrical potential),

2. slow kinetics of reaction (varies with temperature), and

3. junction potentials, or poor electrical contacts.

Problem 3 usually generates a systematic error in all measurements, but the errors should be different for different electrochemical cells or equipment designs.

1.3.2. Calculation of Estimated Thermophysical Properties of Rocks and Minerals: Heat Capacity, Relative Enthalpy, and Calorimetric Entropy of Silicate Minerals and Specific Heat of Silicate Rocks

1.3.2.1. Introduction

The heat capacity of rocks and minerals must be known to evaluate data on both thermochemical and thermophysical properties. The heat capacity of minerals is needed to describe their entropy, enthalpy, and Gibbs energy properties as a function of temperature. The specific heats of minerals and rocks are needed to evaluate data on thermal diffusivity and to calculate thermal diffusivity as a function of temperature.

The experimental heat capacity measurements are lacking, inadequate, or unreliable for many minerals and for most rocks. In these cases, the heat capacity and calorimetric entropy must be estimated.

The standard molar heat capacity and calorimetric entropy of minerals at temperatures greater than 298 K have often been approximated by summing, in appropriate proportions, the standard molar heat capacity and calorimetric entropy of their constituent oxide formula groups. The realization that the heat capacity of most substances is approximately equal to the sum of the heat capacities of its constituent oxides or elements is quite old and can be traced back to a relationship proposed by Kopp (1864). More accurate estimates often can be obtained by a mineral summation technique, in which the standard molar heat capacity or entropy of reaction among oxides and silicates of similar structural class is assumed to be zero or a function of atomic mass, ionic size and charge, and/or molar volume (Helgeson and others, 1978; Nriagu, 1975; Saxena, 1976; Cantor, 1973, 1977; Latimer, 1952).

The general validity of any of these approaches is rooted in the fact that lattice vibrational modes are the dominant contribution to heat capacity and calorimetric entropy. To the degree that silicate mineral structures can be approximated as oxygen frameworks with vibrating interstatial cations, the overall lattice modes will be largely a function of the modes of the individual cation-oxygen polyhedra. It is this feature which allows the spectroscopist to identify both the coordination and composition of components in mineral phases from their spectral characteristics. This relationship also implies that the standard molar heat capacity and calorimetric entropy of minerals can be estimated by summing, in appropriate proportions, fictive molar heat capacities and calorimetric entropies for the constituent structural groups in minerals.

The fictive molar heat capacities and fictive molar entropies are the average molar heat capacities and molar entropies of a component

in a given coordination within the oxygen framework on the phases. Under this definition, Mg in 4-fold, 6-fold, and 8-fold coordination are listed as MgO-4, MgO-6, and MgO-8, respectively. The heat capacity and calorimetric entorpy contribution of each component were found by least-squares evaluation as will be described below.

However, the reader should be cautioned against drawing conclusions regarding possible fictive spectra for any of the fictive components present here. While measured spectra can be integrated to supply reasonable estimat of heat capacity and entropy (Kieffer, 1979a, 1979b, 1979c, 1980), the nature of the inverse relationship indicates that heat capacity alone supplies, at best, only poor constaints on the possible vibrational modes. This approach offers several advantages over other estimation techniques. The following problems with the other estimation techniques are eliminated:

1. The mineral summation techniques are path dependent. Results differ depending upon the specific minerals in structural classes which are used to derive estimates.

2. The mineral summation technique produces discontinuities in the estimated heat capacity whenever phases in the summation have a lambda transition or phase inversion in the temperature interval of interest.

The following improvements are offered:

1. improved accuracy relative to oxide-summation or mineral-summation techniques because the coordination of the cation is accounted for,

2. the ability to estimate heat capacity and calorimetric entropy even through data on representative minerals in similar structural

classes is not available, and

3. anomalies in the properties of reference phases or in the oxides have been removed through averaging over a large body of data.

1.3.2.2. Evaluation of fictive molar properties

1.3.2.2.1. Introduction

Fictive molar heat capacities and fictive molar entropies are the average molar heat capacities and molar entropies of an oxide component in a given coordination within the oxygen framework of the phase. Under this definition, Mg in 4-fold, 6-fold, and 8-fold coordination are listed as MgO-4, MgO-6, and MgO-8, respectively. They are assumed to have different contributions to the heat capacity or entropy of the phases in which they are found. The values for each were found by least-squares evaluation as will be described below.

1.3.2.2.2. Fitting procedure

The heat capacity and entropy properties of the fictive structural components of mineral phases have been evaluated following the procedure described by Haas and Fisher (1976) and Haas (1974). The approach and procedure given there have been followed closely and will not be described here in detail. A description summarizing the evaluation procedure can be found in section 1.3.3.2.1.

The mathematical model used in the evaluation of the fictive component properties is based on equation 8 for the heat capacity of mineral phases at constant pressure.

$$C_{p(\text{phase a})} = \sum_i N_i \, \acute{C}_{p,i} \qquad (8)$$

where: N_i represents the stoichiometric coefficient of the ith fictive structural component in mineral phase a; and

$C'_{p,i}$ represents the heat capacity function for the ith fictive structural component (the superscript (′) is used here to denote properties of the fictive components);

$$C'_{p,i} = a_{1,i}/T^2 + a_{3,i}/T^{1/2} + a_{5,i} + 2a_{6,i}T + a_{7,i}T^2 \quad (9)$$

where: $a_{1,i}$, $a_{3,i}$, $a_{5,i}$, $a_{6,i}$, and $a_{7,i}$ are coefficients fitted to the fictive structural component and T is temperature in kelvins.

Equation 9 is a restatement of equation 6 in Haas and Fisher (1976).

The mathematical model used in regression step to fit relative enthalpy is based on the thermodynamic identity

$$H_T(\text{phase b}) - H_{T_r}(\text{phase a}) = \int_0^T C_p(\text{phase b})\, dT - \int_0^{T_r} C_p(\text{phase a})\, dT$$

In the case where phases a and b are identical, the mathematical model used to fit relative enthalpy is

$$(H_T - H_{T_r})(\text{phase a}) = \sum_i N_i\, (H'_{T,i} - H'_{T_r,i}) \quad (10)$$

where: N_i represents the stoichiometric coefficient of the ith structural component in mineral phase a, and

$(H'_{T,i} - H'_{T_r,i})$ represents the relative enthalpy contribution of the ith fictive structural component.

$$(H_{T,i}^{f} - H_{T_r,i}^{f}) = a_{1,i}\left(\frac{1}{T} - \frac{1}{T_r}\right) + 2a_{3,i}\,(T^{1/2} - T_r^{1/2}) +$$

$$a_{5,i}\,(T - T_r) + a_{6,i}\,(T^2 - T_r^2) + \frac{1}{3}\,a_{7,i}\,(T^3 - T_r^3) \qquad (11)$$

where: T_r represents the reference temperature of the relative enthalpy measurement.

In the case where phases a and b are not identical (a phase inversion occurs during the measurement process), the mathematical model used to fit relative enthalpy is

$$(H_T(\text{phase a}) - H_{T_r}(\text{phase b})) = \Delta H_r + \sum_i N_i\,(H_{T,i}^{f} - H_{T_r,i}^{f}) \qquad (12)$$

where: ΔH_r is the enthalpy of reaction of phase b to phase a, and the other terms are the same as in equations 10 and 11.

Equation 12 is valid because, for all phases studied to date, phase inversions rapid enough to occur during a drop calorimetry measurement do not involve a change in structural components but involve a change in the organization of structural components.

The mathematical model used in the regression step to fit calorimetric entropy (at 298.15 K) is

$$(S_T - S_0)(\text{phase a}) = \sum_i N_i\,S_i^{f} \qquad (13)$$

where: N_i represents the stoichiometric coefficient of the ith fictive structural component in mineral phase a, and S_i^{f} represents the calorimetric entropy contribution of the ith fictive structural component.

$$S_i' = -\frac{1}{2}a_{1,i}/T^2 - 2a_{3,i}/T^{1/2} + a_{4,i} + a_{5,i} \ln T + 2a_{6,i} T + \frac{1}{2} a_{7,i} T^2 \quad (14)$$

Equations 9, 11 and 14 are smoothing functions and have no theoretical basis beyond the thermodynamic identities shown in equations 1 and 2. In our work, data at temperatures below 200 K were not considered. Above 200 K, the functions readily describe most data. In order to avoid overfitting of the data, nonsignificant constants have been eliminated from the general equation wherever they were not needed to describe the properties of a phase or fictive component. This is particularly common for the $a_7 T^2$ term in equation 9. Removal of this term eliminated any rapid excursions of the calculated values in the temperature region around and above the highest experimental temperature. Equations 9, 11, and 14 have been fit within the temperature range represented for each fictive structural component and should not be extended indiscriminately to higher or lower temperatures.

Haas (1974) described the mechanics used to fit the model to discrete experimental observations in detail. A description of the typical problem setup is given in section 1.3.3.3.

Data were weighted by the reciprocal of the precision; the higher (smaller in magnitude) the precision, the higher (larger in magnitude) the weight. The use of weighting served two purposes. First, it allowed the simultaneous fitting of different properties that have large variations in magnitude. An example is the simultaneous fitting of relative enthalpy data that could exceed 7 megajoules/mol and heat capacity data that are generally less than 1 kilojoule/mol-K. Second,

weighting constrained the solution towards the more precise observations. This was particularly desirable where precise data from low-temperature, adiabatic calorimetry were being matched with the less precise data from differential scanning calorimetry or from drop calorimetry.

The author's stated precision was used in the first fitting of a data set from a particular reference. In subsequent cycles this would be modified if logic or other data showed the author's estimate to be abnormally small.

1.3.2.2.3. Results

The data used in the evaluation of the fictive component properties is summarized in table 2. Table 3 lists the structural components for common silicate minerals. Table 4 gives the coefficients for the heat-capacity function, equation 9, and for the entropy function, equation 14. They are given for the 20 different fictive components allowed in this study. Figure 1a and b contrast the standard errors of estimate for 86 data sets using the fictive molar heat-capacity summation and the oxide heat-capacity summation, respectively. The dashed lines represent a 2-percent error of estimate for the data sets. On figure 1a, only 15 sets, a little more than 17 percent, lie outside the 2-percent brackets. On figure 1b, 35 sets, a little less than 41 percent, lie outside the 2-percent bracket. Clearly, an estimate using the summation of the fictive component heat capacities is a significant improvement over a summation using the oxide heat capacities. Because the mineral-summation technique of Helgeson and others (1978) is pathdependent, a similar analysis is not available.

Table 2. Experimental (and evaluated) data used to develop the functions for the fictive components

Phase	Property	No. of observations	Temperature range (K)	Reference
Akermanite	relative enthalpy	27	357-1605	Pankratz and Kelley, 1964a
	entropy	1	298	Robie and others, 1979
Albite	apparent specific heats	14	373-1373	White, 1919
	relative enthalpy	5	472-1270	Kelley and others, 1953
	entropy	1	298	Robie and others, 1979
Analbite	apparent specific heats	14	373-1373	White, 1919
	relative enthalpy	5	472-1270	Kelley and others, 1953
	heat capacity	75	339-997	Hemingway and others, 1981
	heat capacity	20	200-370	Openshaw and others, 1976
Analcite	heat capacity	11	206-298	King, 1955
	entropy	1	298	Robie and others, 1979
Andalusite	heat capacity	10	206-296	Todd, 1950
	relative enthalpy	13	397-1601	Pankratz and Kelley, 1964b
	entropy	1	298	Robie and others, 1979
Anorthite	heat capacity	95	349-986	Krupka and others, 1979
	heat capacity	49	202-381	Robie and others, 1978
	apparent specific heats	1/	373-1673	White, 1919
	relative enthalpy	15	400-1800	Ferrier, 1969
	entropy	1	298	Robie and others, 1979
Anthopyllite	heat capacity	36	200-700	Krupka, 1982
	entropy	1	298	Krupka, 1982

Phase	Property	No. of observations	Temperature range (K)	Reference
Antigorite	heat capacity	10	206-296	King and others, 1967
	relative enthalpy	11	405-847	King and others, 1967
Bredigite	relative enthalpy	12	974-1690	Coughlin and O'Brien, 1957
Brucite	heat capacity	21	216-320	Giauque and Archibald, 1937
	entropy	1	298	Robie and others, 1979
	relative enthalpy	12	350-699	King and others, 1975
Ca-Olivine	heat capacity	10	206-296	King, 1957
	relative enthalpy	18	405-1112	Coughlin and O'Brien, 1957
	entropy	1	298	Robie and others, 1979
Ca-Al Clinopyroxene	heat capacity	16	298-1000	Thompson and others, 1978
	heat capacity	50	199-379	H.T. Haselton, unpublished data
	entropy	1	298	Robie and others, 1979
Ca_2SiO_4, alpha	relative enthalpy	5	1714-1816	Coughlin and O'Brien, 1957
Ca_3SiO_5	heat capacity	9	206-296	Todd, 1951
	relative enthalpy	7	573-1773	Gronow and Schweite, 1933
Chrysotile	heat capacity	10	206-296	King and others, 1967
Clinoenstatite	heat capacity	14	298-1600	Robie and others, 1979
	heat capacity	9	215-295	Kelley, 1943
	relative enthalpy	13	580-1570	Wagner, 1932
	entropy	1	298	Robie and others, 1979

Table 2. Continued

Phase	Property	No. of observations	Temperature range (K)	Reference
Cristobalite, alpha	heat capacity	6	200-700	Robie and others, 1979
	entropy	1	298	Robie and others, 1979
Cristobalite, beta	heat capacity	17	400-2000	Robie and others, 1979
Cyclowollastonite	heat capacity	7	201-295	Wagner, 1932
	relative enthalpy	12	576-1558	Wagner, 1932
	apparent specific heats	28	373-1673	White, 1919
	specific heat	6	194-298	Parks and Kelley, 1926
Analcite (dehydrated)	heat capacity	10	206-296	King and Weller, 1961b
	relative enthalpy	9	407-997	Pankratz, 1968
	entropy	1	298	Robie and others, 1979
Diaspore	heat capacity	19	340-509	Krupka, 1982
	heat capacity	10	206-295	King and Weller, 1961a
	heat capacity	215	203-345	Perkins and others, 1979
	heat capacity	15	312-585	Mukaibo and others, 1969
	entropy	1	298	Robie and others, 1979
Dickite	heat capacity	10	206-296	King and Weller, 1961a
Diopside	heat capacity	14	298-1600	Robie and others, 1979
	heat capacity	29	298-1000	Krupka and others, 1980
	relative enthalpy	15	599-1576	Wagner, 1932
	entropy	1	29	Robie and others, 1979
Epidote	relative enthalpy	10	335-1100	Kiseleva and others, 1974

Table 2. Continued

Phase	Property	No. of observations	Temperature range (K)	Reference
Fayalite	heat capacity	31	208-381	Robie and Hemingway, in review
	relative enthalpy	13	395-1370	Orr, 1953
	entropy	1	298	Robie and others, 1979
Fluorphlogopite	heat capacity	10	206-296	Kelley and others, 1959
	relative enthalpy	12	400-1499	Kelley and others, 1959
	entropy	1	298	Robie and others, 1979
Forsterite	heat capacity	9	206-295	Kelley, 1943
	relative enthalpy	16	398-1807	Orr, 1953
	entropy	1	298	Robie and others, 1979
Gehlenite	heat capacity	10	206-296	Weller and Kelley, 1963
	relative enthalpy	15	402-1801	Pankratz and Kelley, 1964a
	entropy	1	298	Robie and others, 1979
Gibbsite	heat capacity	23	200-479	Hemingway and others, 1977
	heat capacity	10	205-296	Shomate and Cook, 1946
	relative enthalpy	5	322-423	Shomate and Cook, 1946
Grossular	heat capacity	1	298	Haselton and Westrum, 1979
	heat capacity	50	350-978	Krupka and others, 1979
	heat capacity	57	200-596	Westrum and others, 1979
	entropy	1	298	Haselton and Westrum, 1979
Halloysite	heat capacity	10	206-296	King and Weller, 1961a
High Sanidine	apparent specific heats	14	373-1373	White, 1919

Table 2. Continued

Phase	Property	No. of observations	Temperature range (K)	Reference
High Sanidine (continued)	heat capacity	69	339-997	Hemingway and others, 1981
	heat capacity	20	200-370	Openshaw and others, 1976
Jadeite	heat capacity	10	206-296	Kelley and others, 1953
	heat capacity	11	298-1300	Robie and others, 1979
	entropy	1	298	Robie and others, 1979
Kaliophilite	heat capacity	10	206-296	Kelley and others, 1953
	relative enthalpy	23	409-1799	Pankratz, 1968
Kaolinite	heat capacity	27	340-800	Hemingway and others, 1978
	heat capacity	10	206-296	King and Weller, 1961a
	entropy	1	298	Robie and others, 1979
Kyanite	heat capacity	10	206-296	Todd, 1950
	relative enthalpy	12	390-1503	Pankratz and Kelley, 1964b
	entropy	1	298	Robie and others, 1979
Larnite	heat capacity	10	206-296	Todd, 1951
	relative enthalpy	10	406-964	Coughlin and O'Brien, 1957
	entropy	1	298	Robie and others, 1979
Lawsonite	heat capacity	16	206-296	King and Weller, 1961b
	heat capacity	8	298-600	Perkins and others, 1980
	entropy	1	298	Robie and others, 1979
Leonhardite	heat capacity	10	206-296	King and Weller, 1961b
	entropy	1	298	Robie and others, 1979

Table 2. Continued

Phase	Property	No. of observations	Temperature range (K)	Reference
Leucite	heat capacity	10	206-296	Kelley and others, 1953
	relative enthalpy	21	409-1798	Pankratz, 1968
	entropy	1	298	Kelley and others, 1953
Low Albite	heat capacity	75	339-997	Hemingway and others, 1981
	heat capacity	20	200-370	Openshaw and others, 1976
	entropy	1	298	Robie and others, 1979
Margarite	heat capacity	24	200-1000	Perkins and others, 1980
	entropy	1	298	Haas and others, 1980
Merwinite	relative enthalpy	17	397-1601	Pankratz and Kelley, 1964a
	entropy	1	298	Robie and others, 1979
Microcline	heat capacity	69	339-997	Hemingway and others, 1981
	heat capacity	20	200-370	Openshaw and others, 1976
	apparent specific heats	14	373-1373	White, 1919
	entropy	1	298	Robie and others, 1979
Muscovite	heat capacity	62	332-967	Krupka and others, 1979
	heat capacity	30	202-385	Robie and others, 1976
	entropy	1	298	Robie and others, 1979
$Na_2Si_2O_5$	relative enthalpy	20	367-1164	Naylor, 1945
Nepheline	heat capacity	10	206-296	Kelley and others, 1953
	entropy	1	298	Kelley and others, 1953

Table 2. Continued

Phase	Property	No. of observations	Temperature range (K)	Reference
Orthoenstatite	heat capacity	151	318-999	Krupka and others, 1980
	entropy	1	298	Krupka and others, 1980
Paragonite	heat capacity	82	200-759	Robie and Hemingway, in review
	entropy	1	298	Robie and Hemingway, in review
Phlogopite	entropy	1	298	Robie and others, 1979
Prehnite	heat capacity	8	200-298	Perkins and others, 1980
	heat capacity	12	298-800	Perkins and others, 1980
	entropy	1	298	Haas and others, 1980
Pyrope	heat capacity	9	264-345	Haselton and Westrum, 1980
	heat capacity	8	298-1000	Robie and others, 1979
	entropy	1	298	Haselton and Westrum, 1980
Pyrophyllite	heat capacity	20	200-370	Robie and others, 1976
	heat capacity	48	335-679	Krupka and others, 1979
	entropy	1	298	Robie and others, 1979
Quartz, alpha	heat capacity	5	200-600	Robie and others, 1979
	entropy	1	298	Robie and others, 1979
Quartz, beta	heat capacity	4	900-1200	Robie and others, 1979
Rankinite	heat capacity	10	206-296	King, 1957

Table 2. Continued

Phase	Property	No. of observations	Temperature range (K)	Reference
Sillimanite	heat capacity	10	206-296	Todd, 1950
	relative enthalpy	13	401-1496	Pankratz and Kelley, 1964b
	entropy	1	298	Robie and others, 1979
Talc	heat capacity	13	200-300	Robie and Stout, 1963
	heat capacity	6	298-800	Robie and others, 1979
	heat capacity	26	298-650	Krupka and others, 1977
	entropy	1	298	Robie and others, 1979
Tremolite	heat capacity	9	298-1100	Robie and others, 1979
	heat capacity	21	298-800	Krupka and others, 1977
	entropy	1	298	Robie and others, 1979
Wollastonite	heat capacity	2	200-210	Cristescu and Simon, 1934
	heat capacity	7	199-303	Christescu, 1931
	heat capacity	137	205-999	Krupka and others, 1980
	relative enthalpy	5	573-1373	Gronow and Schweite, 1933
	relative enthalpy	13	484-1294	Southard, 1941
	relative enthalpy	7	323-1157	Roth and Bertram, 1929
	apparent specific heat	18	373-1573	White, 1919
	relative enthalpy	11	566-1383	Wagner, 1932
	entropy	1	298	Robie and others, 1979
Zoisite	heat capacity	8	200-300	Perkins and others, 1980
	heat capacity	11	298-730	Perkins and others, 1980
	entropy	1	298	Haas and others, 1980

Table 3. Structural factors for common silicate minerals

Mineral group/components	Coordination number	Discussion
1. Olivine group - A_2SiO_4		
A site - Mg^{+2}, Fe^{+2}, Ni^{+2}, Ca^{+2}, Mn^{+2}	6	
SiO_2 site	4	
2. Garnet group - $A_3B_2Si_3O_{12}$		
A site - Ca^{+2}, Fe^{+2}, Mg^{+2}, Mn^{+2}	8	
B site - Al^{+3}, Fe^{+3}, Mn^{+3}	6	
SiO_2 site	4	
3. Mica group - $W_{0-1}Y_{2-3}(Z_4O_{10})(OH)_2$		
W site - K^{+1}, Na^{+1}, Ca^{+2}, H_3O^{+1}	8-12*	*Coordination number of 8 used for Na and Ca, 8 used for K in muscovite, and 6 used for K in phlogopite in evaluation of component properties.
Y site - Al^{+3}, Fe^{+2}, Mg^{+2}, Fe^{+3}	6	
Z site - Si^{+4}, Al^{+3}	4	
OH site - hydroxyl	-	
4. Silica polymorphs - SiO_2, quartz, tridymite, cristobalite		
SiO_2	4	
5. Feldspar group - XZ_4O_8		
X site - K^{+1}, Na^{+1}, Ca^{+2}	6-9*	*7 used.
Z site - Si^{+4}, Al^{+3}	4	
6. Pyroxenoid group - $A_2Z_2O_6$		
A site - Ca^{+2}, Fe^{+2}, Mg^{+2}	6	
Z site - Si^{+4}	4	

Table 3. Continued

Mineral group/components	Coordination number	Discussion
7. Pyroxene group - ABZ_2O_6 (C2/C symmetry)		
A site - Ca^{+2}, Na^{+1}	8	
A site - Mg^{+2}, Fe^{+2}	6	
B site - Mg^{+2}, Fe^{+2}, Al^{+3}	6	
Z site - Si^{+4}, Al^{+3}	4	
8. Kaolinite group - $M_{2-3}Z_2O_5(OH)_4$		
M site - Al^{+3}, Mg^{+2}, Fe^{+2}, Fe^{+3}	6	
Z site - Si^{+4}, Al^{+3}	4	
OH site - hydroxyl	-	
9. Aluminosilicate minerals - $ABSi_2O_5$ (andalusite, kyanite, sillimanite)		
A site - Al^{+3}	4, 5, 6*	*Coordination numbers of 4, 5, and 6 used for sillimanite, andalusite, and kyanite, respectively.
B site - Al^{+3}	6	
SiO_2 site	4	

Table 4. Component coefficients to estimate mineral heat capacity and entropy (joules/mol.-kelvin)

Component	a_1	a_3	a_4	a_5	a_6	a_7
Al_2O_3-4*1	0.00000D+00	-1.37221D+03	-9.92000D+02	1.56985D+02	6.34774D-03	0.00000D+00
Al_2O_3-5	0.00000D+00	-2.08406D+03	-1.34963D+03	2.05756D+02	-7.82311D-03	0.00000D+00
Al_2O_3-6	0.00000D+00	-2.46456D+03	-1.50724D+03	2.22740D+02	-8.20451D-03	0.00000D+00
CaO-6	0.00000D+00	-6.22865D+02	-4.80538D+02	7.88255D+01	-1.91875D-03	0.00000D+00
CaO-7	0.00000D+00	-6.22865D+02	-4.71709D+02	7.88255D+01	-1.91875D-03	0.00000D+00
CaO-8	1.96615D+04	-7.16401D+02	-5.15167D+02	8.36079D+01	-2.97891D-03	0.00000D+00
Fe_2O_3-4/6	4.17088D+05	-3.30795D+03	---------*2	3.18412D+02	-4.89380D-02	2.57115D-05
FeO-6	0.00000D+00	-6.51941D+02	-4.85209D+02	8.11612D+01	0.00000D+00	0.00000D+00
fluorine	0.00000D+00	0.00000D+00	-5.22387D+01	1.39627D+01	1.28265D-02	0.00000D+00
hydrate	0.00000D+00	-2.63847D+02	-3.00702D+02	5.69125D+01	0.00000D+00	0.00000D+00
hydroxyl	6.32070D+05	-1.64532D+03	-8.86693D+02	1.29124D+02	-6.01221D-03	0.00000D+00
K_2O-8	0.00000D+00	6.56875D+02	1.08368D+02	7.71711D+00	5.27163D-02	0.00000D+00
K_2O-6	0.00000D+00	1.71435D+02	-1.25937D+02	4.24609D+01	1.70942D-02	0.00000D+00
MgO-4	0.00000D+00	0.00000D+00	-2.06902D+02	4.30846D+01	7.44796D-04	0.00000D+00
MgO-6	0.00000D+00	-8.72529D+02	-5.88796D+02	8.99331D+01	-3.19321D-03	0.00000D+00

Table 4. Continued

Component	a_1	a_3	a_4	a_5	a_6	a_7
MgO-8	-8.10599D+05	0.00000D+00	-2.45321D+02	4.78300D+01	0.00000D+00	0.00000D+00
Na_2O-6	0.00000D+00	-4.58234D+01	-2.26355D+02	5.80738D+01	1.24598D-02	0.00000D+00
Na_2O-7	0.00000D+00	-4.58234D+01	-2.51172D+02	5.80738D+01	1.24598D-02	0.00000D+00
Na_2O-8	0.00000D+00	-4.58234D+01	-2.59204D+02	5.80738D+01	1.24598D-02	0.00000D+00
SiO_2-4	0.00000D+00	-1.08305D+03	-7.04147D+02	1.09383D+02	-2.77591D-03	0.00000D+00

*1 The number after the "-" in each component name indicates the coordination number of the component.

*2 Stars indicate coefficient value has not been determined.

Figure 1. Plots of the percentage errors for estimates averaged over the temperature range of the data set of the oxide-summation method against the fictive component method for 86 sets of heat-capacity data. Each (+) symbol represents the standard error of estimate, in percent, averaged over the temperature range of each data set used and, therefore, represents as few as one or more than 100 observations. The dashed lines on figure a emphasize 2-percent error for estimates using the fictive component method. The dashed lines on figure b emphasize 2-percent error of estimates using the oxide summation method. Less than half as many sets lie outside of the 2-percent envelope for the fictive component method than do for the oxide summation method.

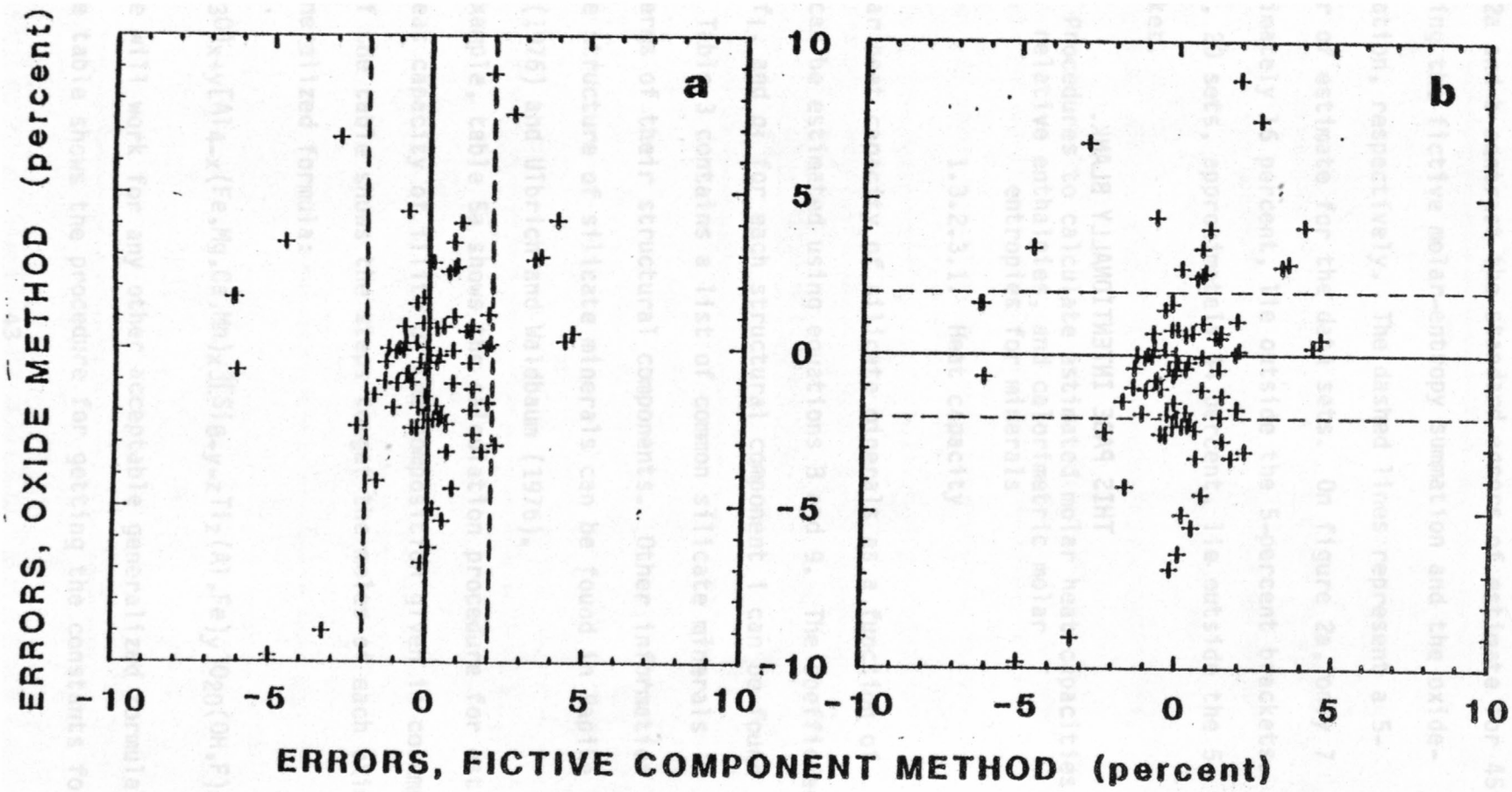
ERRORS, OXIDE METHOD (percent)
a
b
10
5
0
-5
-10
-10
-5
0
5
10
ERRORS, FICTIVE COMPONENT METHOD (percent)

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Figure 2a and b contrast the standard errors of estimate for 45 data sets using the fictive molar-entropy summation and the oxide-entropy summation, respectively. The dashed lines represent a 5-percent error of estimate for the data sets. On figure 2a, only 7 sets, approximately 16 percent, lie outside the 5-percent brackets. On figure 2b, 20 sets, approximately 44 percent, lie outside the 5-percent bracket.

1.3.2.3. Procedures to calculate estimated molar heat capacities, relative enthalpies, and calorimetric molar entropies for minerals

1.3.2.3.1. Heat capacity

The molar heat capacity of silicate minerals as a function of temperature can be estimated using equations 8 and 9. The coefficients a_i, b_i, c_i, f_i, and g_i for each structural component i can be found in table 4. Table 3 contains a list of common silicate minerals defined in terms of their structural components. Other information regarding the structure of silicate minerals can be found in Papike and Cameron (1976) and Ulbrich and Waldbaum (1976).

As an example, table 5a shows the calculation procedure for estimating the heat capacity of illite of the composition given in column 2. Part a of the table shows the steps to get the moles of each oxide using the generalized formula:

$$(K,Na,H_3O)_{x+y}[Al_{4-x}(Fe,Mg,Ca,Mn)_x][Si_{8-y-z}Ti_z(Al,Fe)_y]O_{20}(OH,F)_4$$

The procedure will work for any other acceptable generalized formula. Part b of the table shows the procedure for getting the constants for

Figure 2. Plots of the percentage errors for estimates from the oxide summation method against the percentage errors for estimates from the fictive component method for 45 sets of molar calorimetric entropy data at 298.15 K. The dashed lines on figure a emphasize 5-percent error of estimates using the fictive component method. The dashed lines on figure b emphasize 5-percent error of estimates using the oxide summation method. Less than half as many sets lie outside of the 5-percent envelope for the fictive component method than do for the oxide summation method.

Figure 2, Robinson and others

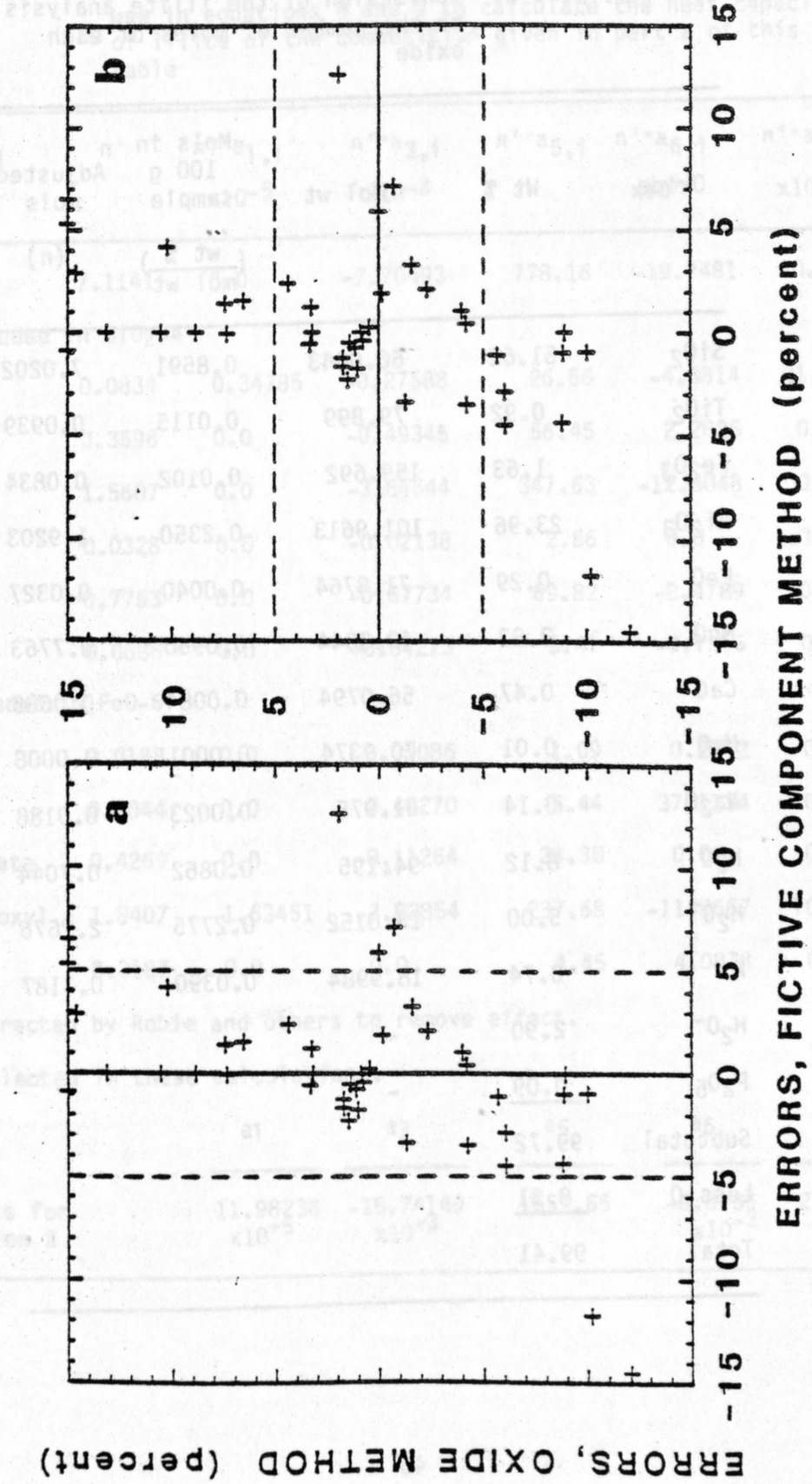


Table 5, part a. Conversion of the illite analysis to the number of moles of each oxide

Oxide	Wt %	Mol wt	Mols in 100 g sample $(\frac{\text{wt \%}}{\text{mol wt}})$	Adjusted mols (n)
SiO_2	51.62	60.0843	0.8591	7.0202
TiO_2	0.92	79.899	0.0115	0.0939
Fe_2O_3	1.63	159.692	0.0102	0.0834
Al_2O_3	23.96	101.9613	0.2350	1.9203
FeO	0.29	71.8764	0.0040	0.0327
MgO	3.83	40.3044	0.0950	0.7763
CaO	0.47	56.0794	0.0084	0.0686
MnO	0.01	70.9374	0.0001	0.0008
Na_2O	0.14	61.975	0.0023	0.0188
K_2O	8.12	94.195	0.0862	0.7044
H_2O^+	5.00	18.0152	0.2775	2.2676
F	0.74	18.9984	0.0390	0.3187
H_2O^-	2.90	-		
P_2O_5	0.09	-		
Subtotal	99.72			
Less O	0.31			
Total	99.41			

Table 5, part b. Calculation of the constants a_1, a_2, a_3, a_6, and a_7 for use in equations 8 and 9 to calculate the heat capacity of illite of the composition given in part a of this table

Structural Component	n'	$n'\cdot a_{1,i}$ $\times 10^{-5}$	$n'\cdot a_{3,i}$ $\times 10^{-3}$	$n'\cdot a_{5,i}$	$n'\cdot a_{6,i}$ $\times 10^{+3}$	$n'\cdot a_{7,i}$ $\times 10^{+5}$
SiO_2-4	7.1141	0.0	-7.70493	778.16	-19.7481	0.0
TiO_2 included in SiO_2-4						
Fe_2O_3-4	0.0834	0.34785	-0.27588	26.56	-4.0814	21.4434
Al_2O_3-4	0.3596	0.0	-0.49345	56.45	2.2826	0.0
Al_2O_3-6	1.5607	0.0	-3.84644	347.63	-12.8048	0.0
FeO-6	0.0328	0.0	-0.02138	2.66	0.0	0.0
MgO-6	0.7763	0.0	-0.67734	69.82	-2.4789	0.0
CaO-6	0.0686	0.0	-0.04273	5.41	-0.1316	0.0
MnO included in FeO-6						
Na_2O-8	0.0188	0.0	-0.00086	1.09	0.2342	0.0
K_2O-12	0.7044	0.0	0.46270	5.44	37.1334	0.0
H_2O hydrate	0.4269	0.0	-0.11264	24.30	0.0	0.0
H_2O hydroxyl	1.8407	1.63451	-3.02854	237.68	-11.0667	10.0
F	0.3187	0.0	0.0	4.45	4.0878	0.0

H_2O^- corrected by Robie and others to remove effect.

P_2O_5 neglected in these calculations.

	a_1	a_3	a_5	a_6	a_7
Constants for equation 2	11.98236 $\times 10^{+5}$	-15.74149 $\times 10^{+3}$	1559.65	-6.5735 $\times 10^{-3}$	21.4434 $\times 10^{-5}$

illite of the cited composition for use in equations 8 and 9, above. The analysis was chosen because 1) Robie and others (1976) used this sample to measure the heat capacity between 15 and 380 K and 2) these data were not used to evaluate the estimation functions given on table 4. The detailed steps for the calculation are as follows:

1. Divide the weight percent (table 5a, column 2) of the oxide in the analysis by the molecular weight of that oxide (table 5a, column 3) to get the number of moles (table 5a, column 4) in a 100-gram sample.

2. If we neglect the alkalis K, Na, and H_3O, the number of cation sites total 12. Again, neglecting the alkalis, the sum of moles of cations in column 4 for the 100 grams of illite is 1.4685. In order to adjust the 100 grams up to be equivalent to the chosen formula, multiply all values in column 3 by (12/1.4685) or 8.17160. These results are shown in column 5. The amount of P_2O_5 and "H_2O-" in the analysis was neglected because the P_2O_5 content was low and because the heat capacities for the illite as given by Robie and others in their table 6 had already been adjusted for the adsorbed water. Part b of table 5 continues the calculation.

3. Column 1 gives the structural components for which there are functions. Column 2 gives the adjusted moles for each of these structural components. Note that there are no structural components for TiO_2 and MnO. These have been approximated by adjusting the moles of SiO_2-4 and FeO-6 respectively. In this analysis, these corrections are minor. Had the TiO_2 or MnO contents of the mineral been a major part, such proxies would not necessarily work.

4. The breakdown between Al_2O_3-4 and Al_2O_3-6 was made such that, after the moles of TiO_2 and twice the moles of Fe_2O_3 were added to the

moles of SiO_2, the balance to make up 8 moles was made up by Al_2O_3-4. The remaining aluminum oxide was calculated as Al_2O_3-6.

5. The breakdown between hydroxyl water and hydronium water was done in a similar fashion. Fluorine will be found in the hydroxyl sites both because of size and of charge. Therefore, the balance to make up 4 moles was accomplished with $n(H_2O)/2$ moles of water. The remaining H_2O was considered to be the hydronium ion H_3O^+ needed to balance the charge.

6. The calculations are rechecked for this mineral by the following. In theory, the sum of moles of the alkali cations should be equal to the number of moles, y, of Al and Fe in Si sites plus the number of moles, x, of Fe, Mg, Ca, and Mn in the Al site. In this analysis, x = 0.886 moles and y = 0.8777 moles. They sum to 1.7637 moles. However, the moles of alkalis sum to [(0.088 + 0.7044)x2 + 0.4269x2/3] or 1.731 moles. There is an alkali deficiency of 0.0327 moles. This is consistent with a chemical analysis for a mineral such as illite. It is not a perfect world. Column 2 of part b contains the adjusted moles n' that are used in further calculations.

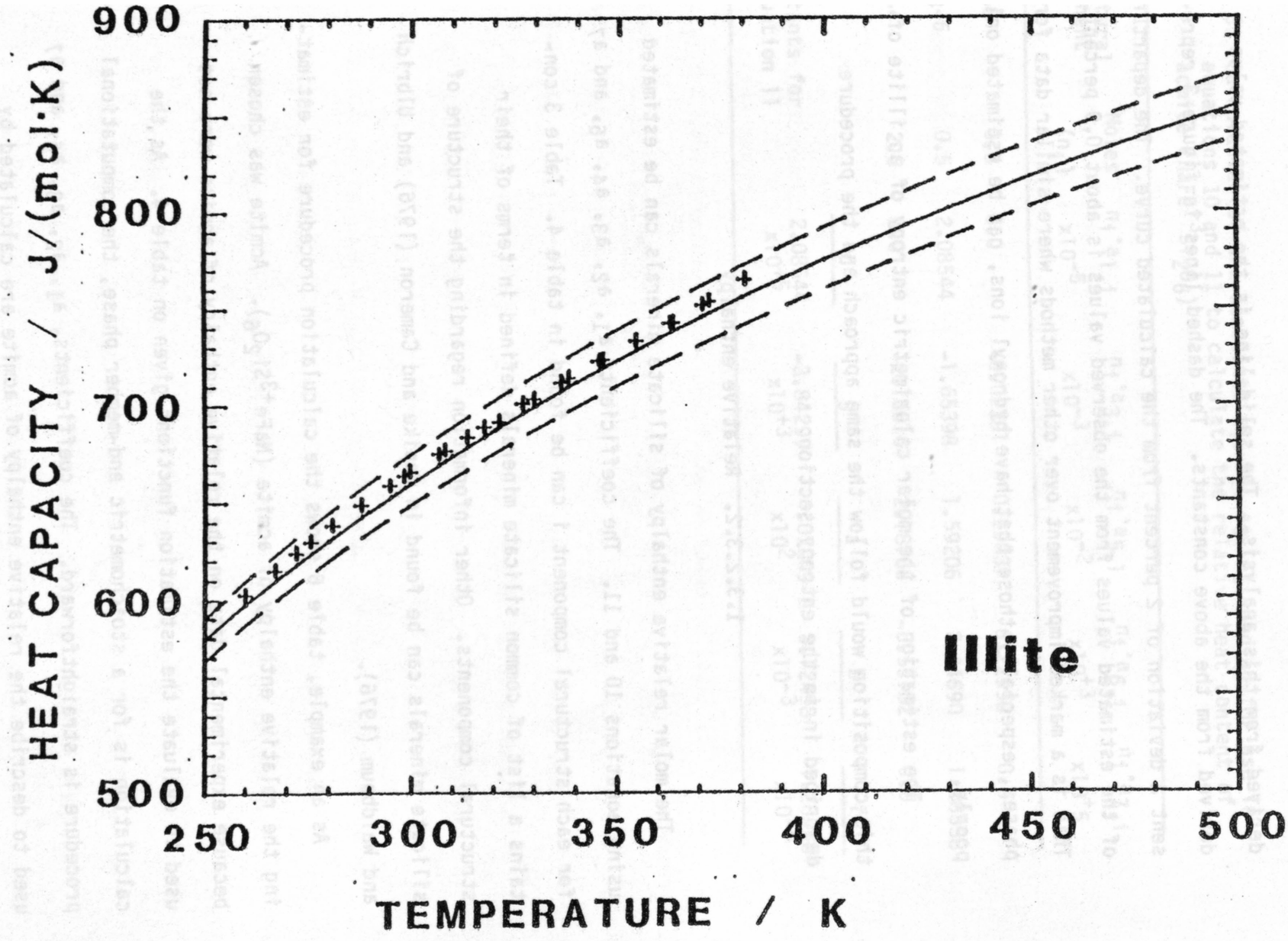
7. Columns 3 through 7 of part b were obtained by multiplying the constants a_1 through a_7 of table 3 by n'.

8. The columns 3 through 7 were summed to get the constants for illite for use in equation 2.

9. The heat capacity of illite at any desired temperature was then calculated.

Figure 3 shows the experimental data of Robie and others (1976) adjusted to the formula weight of 790.39 grams, the formula weight

Figure 3. Plot of the experimental and estimated heat capacities for an illite sample used by Robie and others (1976). They are shown by + and a solid line, respectively. The analysis of the illite is given on table 4a, column 2. The dashed lines represent an error of 2 percent about the estimated heat-capacity function. The function departs from the experimental data by about 0.9 percent.


900
800
700
600
500
HEAT CAPACITY / J/(mol·K)
250
300
350
400
450
500
TEMPERATURE / K
Illite

derived from this analysis. The solid line is the estimated value derived from the above constants. The dashed lines in figure 3 represent a deviation of 2 percent from the calculated curve. The departure of the estimated values from the observed values is about 0.9 percent. This is a marked improvement over other methods where similar data for phases, especially those that have hydroxyl ions, can be estimated only poorly.

The estimation of the molar calorimetric entropy of an illite of this composition would follow the same approach and the procedure described in in the entropy section.

1.3.2.3.2. Relative enthalpy

The molar relative enthalpy of silicate minerals can be estimated using equations 10 and 11. The coefficients a_1, a_2, a_3, a_4, a_6, and a_7 for each structural component i can be found in table 4. Table 3 contains a list of common silicate minerals defined in terms of their structural components. Other information regarding the structure of silicate minerals can be found in Papike and Cameron (1976) and Ulbrich and Waldbaum (1976).

As an example, table 6 shows the calculation procedure for estimating the relative enthalpy of acmite ($NaFe^{+3}Si_2O_6$). Acmite was chosen because experimental data on the relative enthalpy of acmite were not used to evaluate the estimation functions given on table 4. As the calculation is for a stoichometric end-member phase, the computational procedure is straightforward. The coefficients, a_1, a_2, a_3, a_6, and a_7 used to describe the relative enthalpy of acmite are calculated by

Table 6. Calculation of the constants a_1, a_2, a_3, a_6, and a_7 for use in equations 10 and 11 to calculate the relative heat content of acmite ($NaFe^{+3}Si_2O_6$)

Structural Component	Moles (n_i)	$n_i \cdot a_{1,i}$ x10^{-5}	$n_i \cdot a_{3,i}$ x10^{-3}	$n_i \cdot a_{5,1}$ x10^{-2}	$n_i \cdot a_{6,i}$ x10^{+3}	$n_i \cdot a_{7,i}$ x10^{+5}
Na_2O-8	0.5	0.0	-0.02291	0.29037	6.22990	0.0
Fe_2O_3-6	0.5	2.08544	-1.65398	1.59206	2.44690	1.28558
SiO_2-4	2.0	0.0	-2.16610	2.18766	-5.55182	0.0
		c	g	a	b	f
Constants for equation 11		2.08544 x10^{+5}	-3.84299 x10^{+3}	4.07009 x10^{2}	3.12498 x10^{-3}	1.28558 x10^{-5}

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summing the products of the moles of each component i in one mole of acmite and the coefficients, $a_1 \ldots g_7$, for each component i. Figure 4 compares the calculated relative enthalpies with measured relative enthalpies (Ko and others, 1977) for acmite. The dashed lines in figure 4 represent a deviation of 2 percent from the calculated curve. Note that the measured relative enthalpy values lie well within this 2-percent window.

1.3.2.3.3. Entropy

The calorimetric molar entropy of silicate minerals can be estimated using equations 13 and 14. The coefficients a_i, a_3, a_5, a_6, a_7, and g_i for each structural component i can be found in table 4. Table 3 contains a list of common silicate minerals defined in terms of their structural components. Other information regarding the structure of silicate minerals can be found in Papike and Cameron (1976) and Ulbrich and Waldbaum (1976). In addition, Ulbrich and Waldbaum (1976) present structural information on silicate minerals needed to correct calorimetric entropy to third-law entropy.

The general procedure for the estimation of the molar calorimetric entropy for a phase would follow the same approach described in the calculation of estimated heat capacity of illite and relative enthalpy of acmite.

As an example, table 7a shows the calculation procedure to estimate the calorimetric molar entropy of an ideal illite ($K_3Al_7Mg(Si_{14}Al_2)O_{40}(OH)_8$). Measured data on the calorimetric molar entropy of illite was excluded from the evaluation. Table 7b compares the

Figure 4. Plot of experimental and estimated relative enthalpies ($H_T - H_{298.15}$) for acmite ($NaFe^{+3}Si_2O_6$). The estimated values were calculated using equations 5 and 6 and the coefficients listed in table 5 and are shown by a solid line. The dashed lines represent an error of 2 percent about the estimated relative enthalpy function. The experimental measurements of Ko and others, 1977, on a synthetic acmite are shown by x. The function departs from the experimental data by about 0.4 percent.

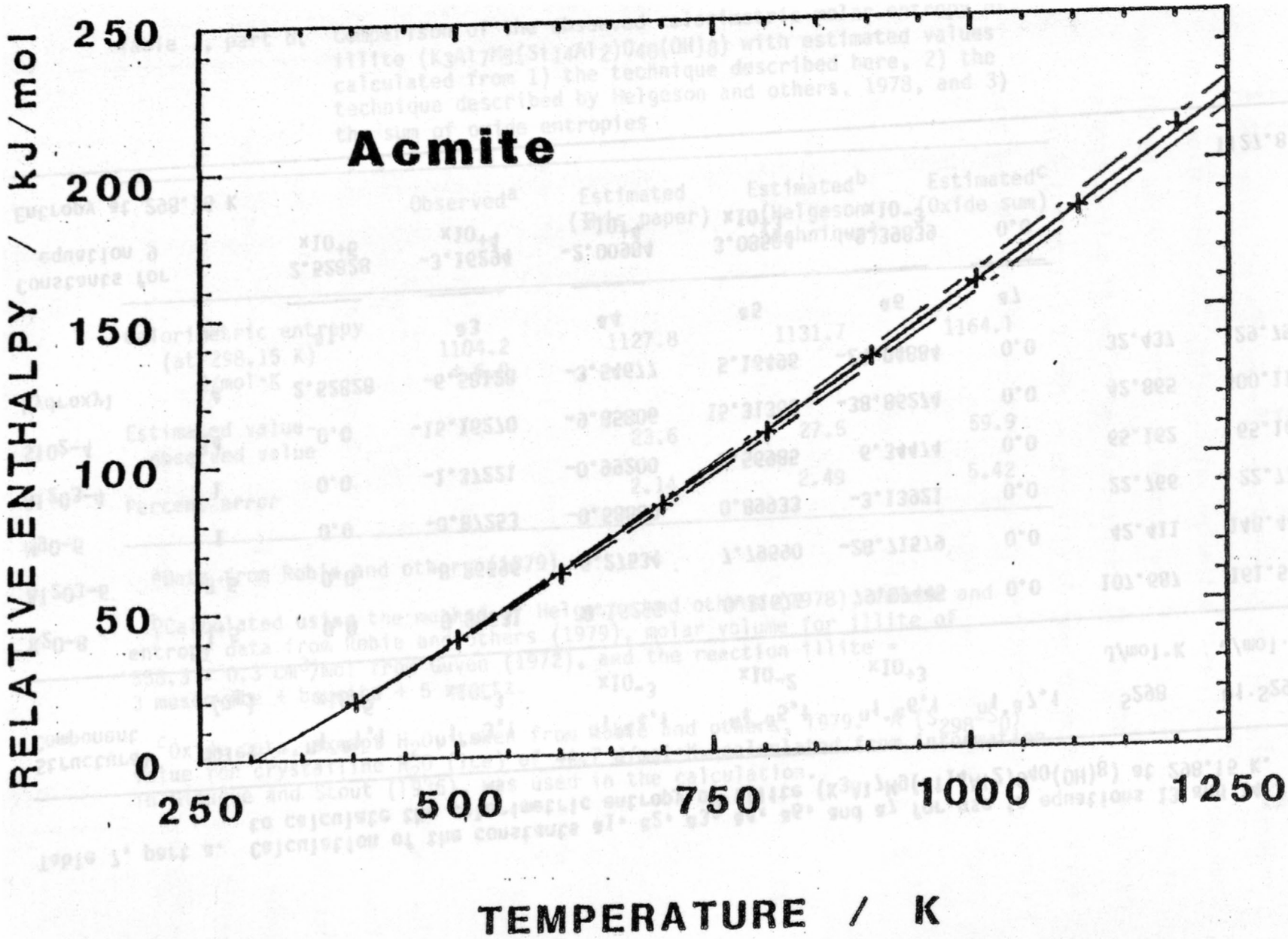

Acmite
RELATIVE ENTHALPY / kJ/mol
250
200
150
100
50
0
250
500
750
1000
1250
TEMPERATURE / K

Table 7, part a. Calculation of the constants a_1, a_2, a_3, a_4, a_6, and a_7 for use in equations 13 and 14 to calculate the calorimetric entropy of illite ($K_3Al_7Mg(Si_{14}Al_2)O_{40}(OH)_8$) at 298.15 K.

Structural Component	Moles (n_i)	$n_i \cdot a_{1,i}$ $\times 10^{-6}$	$n_i \cdot a_{3,i}$ $\times 10^{-3}$	$n_i \cdot a_{4,i}$ $\times 10^{-3}$	$n_i \cdot a_{5,i}$ $\times 10^{-2}$	$n_i \cdot a_{6,i}$ $\times 10^{+3}$	$n_i \cdot a_{7,i}$	S_{298} J/mol·K	$n_i \cdot S_{298}$ J/mol·K
K_2O-8	1.5	0.0	0.98531	0.16255	0.11576	79.07445	0.0	107.687	161.53
Al_2O_3-6	3.5	0.0	-8.26596	-5.27534	7.79590	-28.71579	0.0	42.411	148.44
MgO-6	1	0.0	-0.87253	-0.58880	0.89933	-3.13921	0.0	22.766	22.77
Al_2O_3-4	1	0.0	-1.37221	-0.99200	1.56985	6.34474	0.0	65.162	65.16
SiO_2-4	14	0.0	-15.16270	-9.85806	15.31362	-38.86274	0.0	42.865	600.11
Hydroxyl	4	2.52828	-6.58128	-3.54677	5.16496	-24.04884	0.0	32.437	129.75
		a_1	a_3	a_4	a_5	a_6	a_7		
Constants for equation 9		2.52828 $\times 10^{+6}$	-3.16294 $\times 10^{+4}$	-2.00984 $\times 10^{+4}$	3.08594 $\times 10^{+3}$	-9.39839 $\times 10^{-3}$	0.0		
Entropy at 298.15 K									1127.8

Table 7, part b. Comparison of the observed calorimetric molar entropy of illite ($K_3Al_7Mg(Si_{14}Al_2)O_{40}(OH)_8$) with estimated values calculated from 1) the technique described here, 2) the technique described by Helgeson and others, 1978, and 3) the sum of oxide entropies

	Observed[a]	Estimated (This paper)	Estimated[b] (Helgeson technique)	Estimated[c] (Oxide sum)
Calorimetric entropy (at 298.15 K) J/mol·K	1104.2 ± 6.0	1127.8	1131.7	1164.1
Estimated value-observed value		23.6	27.5	59.9
Percent error		2.14	2.49	5.42

[a]Data from Robie and others (1979).

[b]Calculated using the method of Helgeson and others (1978), volume and entropy data from Robie and others (1979), molar volume for illite of 558.3 ± 0.3 cm^3/mol from Guven (1972), and the reaction illite = 3 muscovite + brucite + 5 quartz.

[c]Oxide data, except H_2O, taken from Robie and others, 1979. A (S_{298}-S_0) value for crystalline H_2O (ice) of 44.7 J/mol·K, calculated from information in Giauque and Stout (1936), was used in the calculation.

observed value for the calorimetric molar entropy of illite (Robie and others, 1976) with estimated values using 1) the estimation technique described here, 2) the estimation technique described by Helgeson and others, 1978, and 3) estimation based on sum of oxide entropies. Our estimated molar entropy of illite at 298.15 K (1127.8 J/mol·K) differs by 2.1 percent from the measured molar entropy (1104.2 ± 6.0 J/mol·K, Robie and others, 1976).

1.3.2.4. Procedure to calculate estimated specific heats for rocks

The specific heat of silicate rocks as a function of temperature can be estimated using the following procedure.

$$\text{rock specific heat (J/g·K)} = \frac{\sum_i X_i C_i}{\sum_i X_i} \qquad (15a)$$

where X_i = (grams of component i in rock)/(grams of rock)

$$C_i = \frac{a_{1,i}}{T^2} + \frac{a_{3,i}}{T^{1/2}} + a_{5,i} + 2a_{6,i}\, T + a_{7,i}\, T^2 \qquad (15b)$$

The coefficients a_1, a_3, a_5, a_6, and a_7 for each component i can be found in table 8. An example of calculations of estimated specific heat for basalt is shown in table 9, based upon the basalt chemistry shown in table 1. A comparison of the estimated specific heats for basalt and measured specific heats for a basalt from Dresser, Wisconsin (Hanley and others, 1977) is shown in table 9.

Table 8. Component coefficients to calculate rock specific heat (joules/gm-kelvin)

	a_1	a_3	a_5	a_6	a_7
SiO_2	0.00000D+00	-1.80210D+01	1.82029D+00	-4.61871D-05	0.00000D+00
TiO_2	0.00000D+00	-1.47083D+01	1.62105D+00	-1.41404D-04	6.59702D-08
Al_2O_3	0.00000D+00	-1.34537D+01	1.53910D+00	6.23640D-05	0.00000D+00
Fe_2O_3	2.61183D+03	-2.07146D+01	1.99391D+00	-3.06452D-04	1.61007D-07
FeO	0.00000D+00	-9.07581D+00	1.12971D+00	0.00000D+00	0.00000D+00
MnO	0.00000D+00	0.00000D+00	5.60685D-01	1.44421D-04	-8.04267D-08
MgO	0.00000D+00	-2.16622D+01	2.23223D+00	-7.94663D-05	0.00000D+00
CaO	0.00000D+00	-1.10740D+01	1.40329D+00	-3.35115D-05	0.00000D+00
Na_2O	0.00000D+00	-4.80940D-01	9.10305D-01	2.14390D-04	0.00000D+00
K_2O	0.00000D+00	1.81573D+00	4.51022D-01	1.81504D-04	0.00000D+00
P_2O_5	0.00000D+00	-4.61346D+00	5.64294D-01	8.30332D-04	-5.20355D-07
hydroxyl	3.55918D+04	-9.17058D+01	7.18335D+00	-3.34688D-04	0.00000D+00
fluorine	0.00000D+00	0.00000D+00	3.68074D-01	3.36682D-04	0.00000D+00

Table 9. Estimated specific heats of averaged Yakima basalt using the composition given in table 1. Measured specific heats of basalt at Dreser, Wisconsin (data from Hanley and others, 1977)

T/C	Estimated specific heat Joules/gm-K (1)[a]	Specific heat[e] calculated from measured relative enthalpy
50	0.8027	0.8090
100	0.8614	0.8689
150	0.9092	0.9200
200	0.9490	0.9617
250	0.9826	0.9932
300	1.0116	1.0110
350	1.0367	
400	1.0588	
450	1.0783	
500	1.0957	

[a]Average Yakima basalt, Waters, 1961 (table 8, part a, column 1)

[b]Data from Hanley and others, 1977

1.3.3. Evaluated Thermodynamic and Thermophysical Properties of Selected Mineral Phases in the MgO-SiO_2-H_2O-CO_2, Fe-FeO-Fe_2O_3-SiO_2, and CaO-Al_2O_3-SiO_2-H_2O-CO_2 Chemical Systems

1.3.3.1. Introduction

The experimental data on the selected phases (Appendix section 1.5.1) in the MgO-SiO_2-H_2O-CO_2, Fe-FeO-Fe_2O_3-SiO_2, and CaO-$Al_2O_3$$SiO_2$-$H_2O$-$CO_2$ chemical systems were evaluated using the method of Haas and Fisher (1976). The goal was to produce a set of thermodynamic properties for each phase at a standard state of 1 atm (101.325 kPa) that is consistent with thermodynamic theory, the observed properties of each phase, and the observed phase relations among the phases. The experimental data used in the study came from a literature search through March 1982.

1.3.3.2. Fitting procedure

1.3.3.2.1. Introduction

The details of the approach and the procedure are described by Haas and Fisher (1976) and by Haas (1974). The approach and procedure given there have been followed closely and will not be described here in detail. The following description summarizes the evaluation procedure:

1. Literature search

   a. Review of literature for data that define thermodynamic properties of a phase or a group of phases.

   b. Close scrutiny of each citation to determine:

      (1) What was physically observed.

      (2) With what precision was it observed.

2. Refinement cycle

a. Comparison of related data (heat capacity, relative enthalpy, enthalpies of formation, enthalpies of reaction, Gibbs energy of reaction, entropies, molar volumes, expansivities, compressibilities) for phases in a chemical system using weighted, simultaneous, multiple, least-squares regression.

b. Review of the pertinent literature where data are found not to be in agreement.

c. Removal of assumed or apparently erroneous data from the set of data being fit by the regression.

d. Repeat of steps a through c until all discordant data have been identified and removed.

3. Preparation of tables using the smoothing functions and the variance-covariance matrix from the last execution of step 2a.

The mathematical model used in the regression in step 2a is based on equation 15 for the heat capacity at constant pressure, equation 16 for molar volume as a function of pressure and temperature, and the known relations among heat capacity, enthalpy, entropy, Gibbs energy and volume for the $\underline{i}$th phase in a group of chemically related phases. The constants $a_{2,i}$ and $a_{4,i}$ were reserved for the constants of integration to describe the enthalpy and entropy of the $\underline{i}$th phase respectively. Equation 15 is a restatement of Haas and Fisher's equation 6:

$$C^{\circ}_{p,i} = \frac{a_{1,i}}{T^2} + \frac{a_{3,i}}{T^{1/2}} + a_{5,i} + 2\,a_{6,i}\,T + a_{7,i}\,T^2 \quad (15)$$

$$V_i^\circ = b_{1,i} + b_{2,i}T + b_{3,i}\exp(-T/300) + b_{4,i}P + b_{5,i}\exp(-P/35000) \quad (16)$$

Equations 15 and 16 have no theoretical basis. They are smoothing functions only and must be so considered! At the absolute zero of temperature equation 15 is indeterminate. In our work, data at temperatures below 200 K were not considered. Above 200 K, the functions readily describe most data. In order to avoid overfitting of the data, nonsignificant constants have been eliminated from the general equation wherever they were not needed to describe the properties of a phase. This is particularly common for the last term, $a_{7,i}T^2$, in equation 15. Removal of this term eliminated any rapid excursions of the calculated values in the temperature region around and above the highest experimental temperature. Equation 15 has been fit within the temperature range presented for each phase in the appendix and should not be extended indiscriminately to higher or lower temperatures.

1.3.3.3. Data entry

Haas (1974) described the mechanics used to fit the model to discrete experimental observations in detail. The typical problem includes the following information:

1. Title for problem.
2. Control codes to identify the options used.
3. Number and labels for the phases in the problem.
4. Sets of data being fit.
   a. Name of the set and reference.

b. Control codes related to the observation and to data editing.

c. Label(s) for the phase(s), the stoichiometric coefficient(s) and any pertinent data on polymorphs.

d. Data as given in the reference.

(1) Temperature (and correction factor if needed to convert to kelvins).

(2) Observed value (and correction factor if needed to convert to joules, volts, moles, etc.).

(3) Precision.

(4) Second independent variable (if needed).

5. Constants of Equation 15 above for each of the reference phases as well as the trial constants for the phases for which the properties are being refined.

6. Control parameters for the error plots.

The input format is designed to reduce manual conversions before entry into the computer for fitting.

The class of data that is not discussed by Haas consists of bracketed observations like those typical of phase equilibria studies. As an example, let us consider reaction A, below.

$$CaAl_2Si_2O_8(\text{anorthite}) + Al_2O_3(\text{corundum}) + H_2O(\text{gas}) = CaAl_4Si_2O_{10}(OH)_2(\text{margarite}) \quad (A)$$

Chatterjee (1974) determined that the equilibrium at 100 MPa was located between 470 and 500°C (743.15 and 773.15 K, respectively). If we consider no additional information, there is an equal probability of equilibrium occurring at any temperature between these two bracketing

temperatures at 100 MPa. Therefore, if we neglect the errors associated with the measurement of temperature and pressure, the probability curve is a square wave whose bounds are at 743.15 K and 773.15 K. To consider the reaction to occur at the midpoint of the bracket, 758.15 K, is unwarranted; this would cause the fitting algorithms to give too much weight to the mid-points of bracketed data. We evaluated the phase equilibrium data by calculating the Gibbs energy of reaction for each two experimentally measured bracketing pressures and temperatures as if each bracketing pressure and temperature represented equilibrium. This procedure does not define a square probability curve between the bracketing values but does define a nearly uniform probability between the bracketing values and allows a sufficient probability of occurrence outside the bracketing values to compensate for errors in measurement of pressure and temperature. The Gibbs energy for the reaction for both bracketing reaction points is calculated using equation 17:

$$\Delta G_r = \sum N_i H_{i}_{T,P,solids} - T \sum N_i S_{i}_{T,P,solids} + N_{gas} G^{gas}_{p_{ref},T} + \int_{P_{ref}}^{P} \frac{N_{gas}}{1000} V(gas)\, dP_T \qquad (17)$$

where N_i is the stoichiometric coefficient for each phase, i, and V is the volume of the gas phase. The factor 1000 is the conversion factor for cm^3/mol to $J/(kPa \cdot mol)$. The integral represents the Gibbs energy difference of the gas between the pressure of observation and the reference pressure, 101.325 kPa. The Gibbs energy difference for H_2O at constant temperature was calculated from data on the P-V-T function proposed by Haar and others (1979).

1.3.3.4. Weighting of experimental data

Data were weighted by the reciprocal of the precision; the higher (smaller in magnitude) the precision, the higher (larger in magnitude) the weight. The use of weighting served two purposes. First, it allowed the simultaneous fitting of different properties that have large variations in magnitude. An example is the simultaneous fitting of enthalpy data that could exceed 7 MJ and electrochemical potentials that are more like 1.0 millivolt. Second, weighting constrained the solution towards the more precise observations. This was particularly desirable where precise data from low-temperature, adiabatic calorimetry were being matched with the less precise data from differential scanning calorimetry or from drop calorimetry.

In the first fitting of a data set from a particular reference, the author's stated precision was used. In subsequent cycles this would be modified <u>if</u> logic or other data showed the author's estimate to be abnormally small.

Weighting of data within the above guideline was straightforward with two exceptions. The first exception is when the author makes many observations of a phenomenon but only reports an average value and the standard deviation. To enter one value, the average value, would underweight the work that went into the determination relative to the significance of discrete measurements on the same or other properties. We <u>arbitrarily</u> overcame this by making three entries: (1) the average value, (2) the average value less the deviation, and (3) the average value plus the deviation. All three entries had a weight equal to the stated standard deviation.

The second exception is related to the treatment of brackets in phase equilibria. As stated in the preceeding section, the Gibbs energy at the experimental pressure for both temperature limits (or at both pressure limits or the combination that defines the bracket) was entered. The weight was calculated from the arbitrary decision that the precision for each bracket was the difference in Gibbs energy for the bracket with the constraint that the magnitude of the assigned precision was equal to or greater than the precision associated with the determination of the temperature (or pressure) of the limit of the bracket. In this fashion, we reduced the tendency of the regression to settle on the midpoint of a bracket. We will return to this point again when we consider the topic of data rejection.

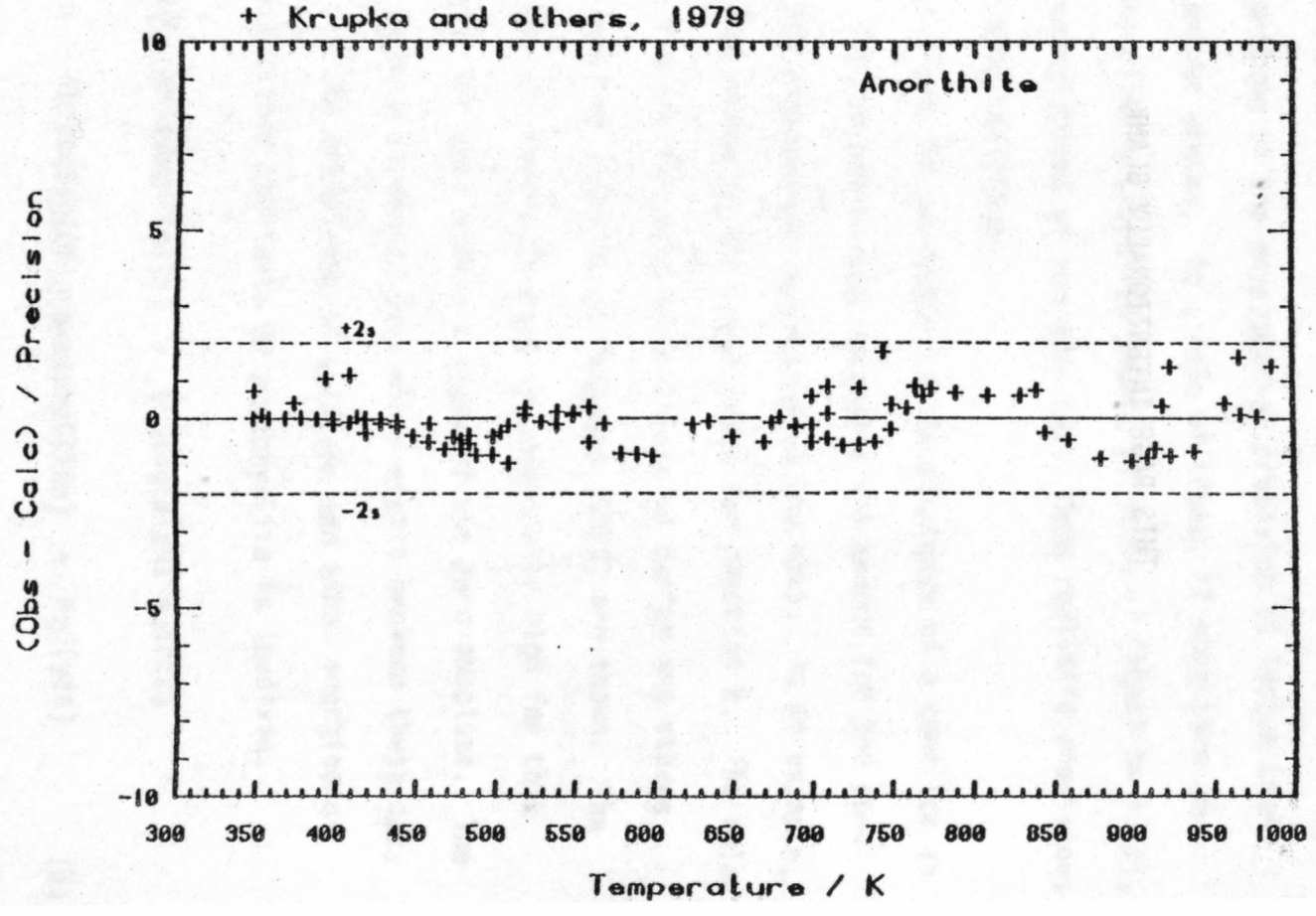
1.3.3.5. Data rejection

Data were rejected during the literature search and during the refinement cycles. Data were rejected during the literature search if there was a clear error in the measurement technique or if there was ambiguity in the identification of the reactants or products.

During the refinement cycle, where all data for all phases in the chemical system are simultaneously fit by the model, the model returns the weighted average of all the data. Error plots such as figure 5 are part of the printed output. On the error plots for each source and type of data, the weighted difference, calculated as (observed-calculated)/precision, is plotted as a function of tempea-ture. These plots give a quick visual picture of the quality of the agreement between the function in the model, the other data in the refinement, and the specific data set. Ideally, the errors should be

Figure 5. Error (observed value - calculated value)/precision as a function of temperature for the differential scanning calorimeter measurements of heat capacity for anorthite. Plus signs (+) indicate the data of Krupka and others, 1979.

Error Plot


+ Krupka and others, 1979
Anorthite
10
5
0
-5
-10
+2s
-2s
(Obs - Calc) / Precision
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
Temperature / K

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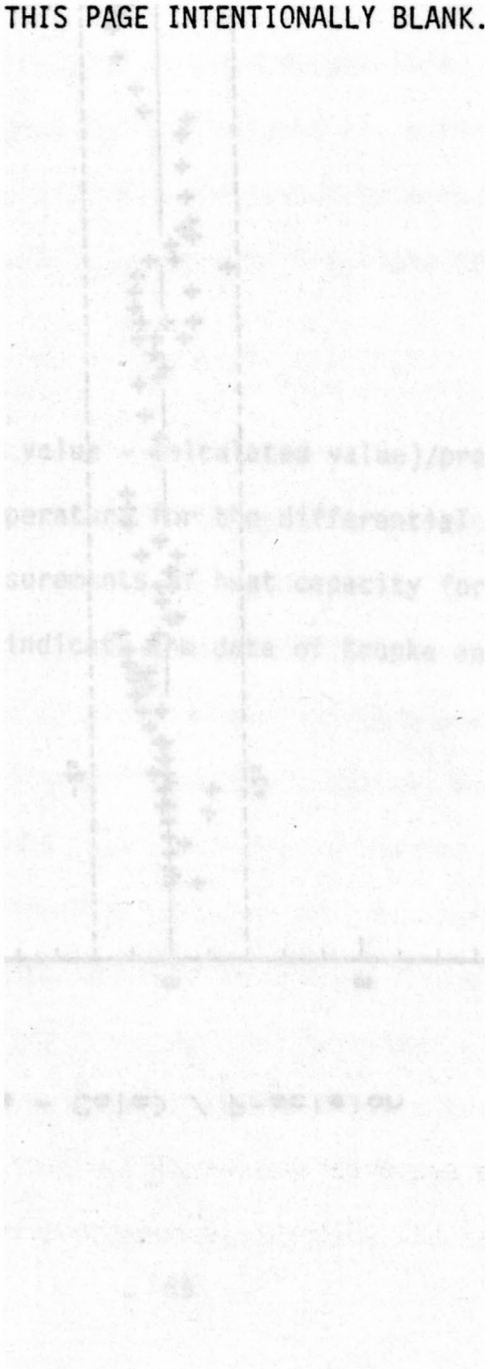


centered about the zero axis and should not exceed ± 2 units (± 2s) of (observed-calculated)/precision. Not attaining such an ideal plot can be the result of one or more of the following:

1. The function does not adequately describe the data.

2. Some set (or sets) of data is not consistent with the balance of the data considered.

3. The magnitude of the experimental precision is larger than that which the author stated. As a rule of thumb, if more than one third of the data plots outside the bounds of +1 to -1 (equal to ± 1s), this leads to overweighting of the data set. More realistic precisions were entered in this situation.

Error plots alert the evaluator to the existence of a conflict in the data sets. The evaluator must determine the source for the conflict and make the appropriate correction to the data. As an example, figure 6 is a combination of the error plots for reaction B. The relative errors for the silicic acid solubilities of Hemley and others (1980) and the reversed brackets of Thompson (1970) are shown. The data of Hemley and his coworkers plot systematically high for this reaction, but they are well within 1 sigma of the zero abscissa. The systematic discrepancy is caused by a minor misfit between these data and one or more of the enthalpies of solution and Gibbs energies of reaction in which either kaolinite or pyrophyllite is involved.

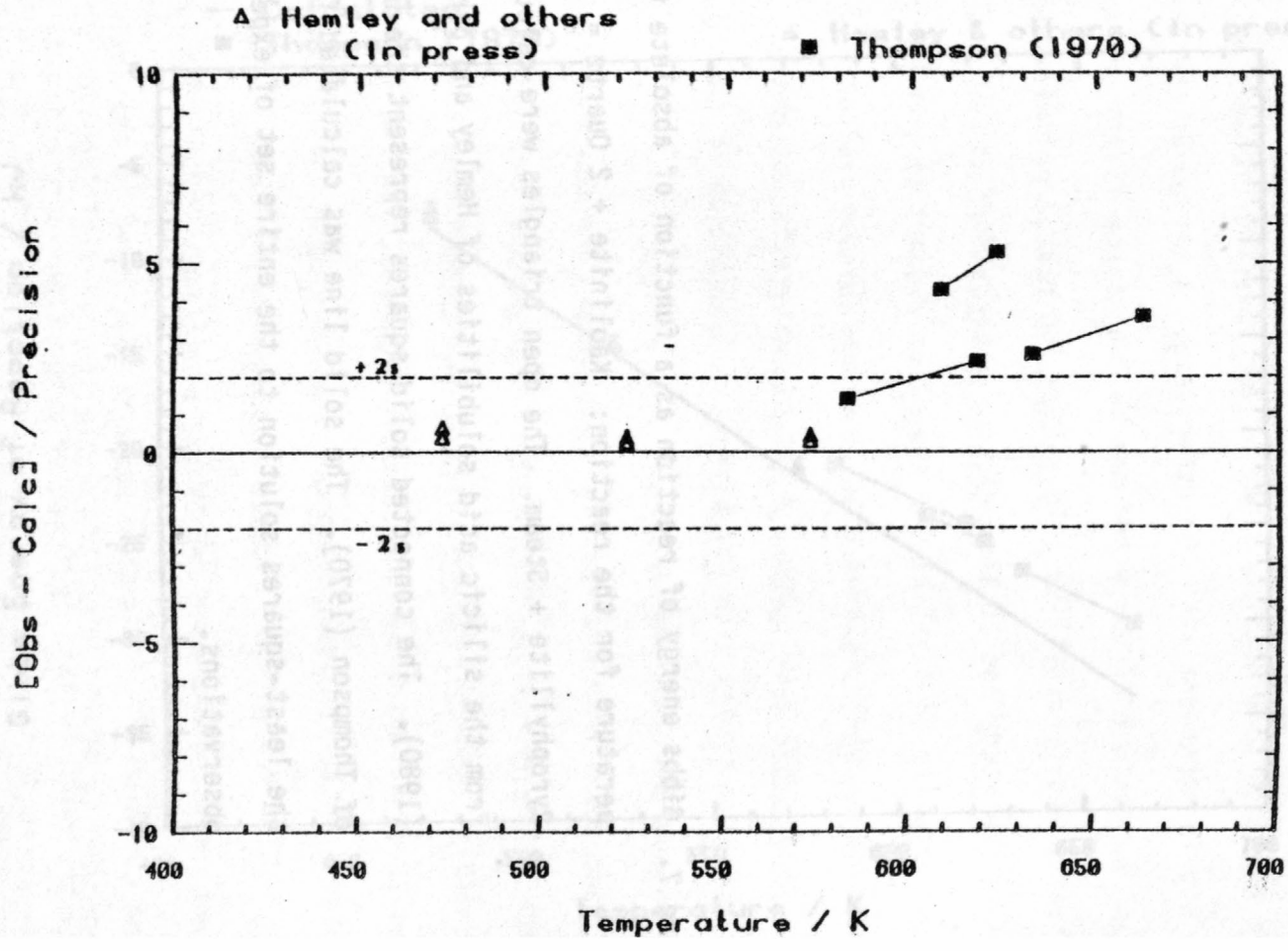
$$Al_2Si_2O_5(OH)_4(\text{kaolinite}) + 6\ SiO_2(\text{alpha quartz})$$

$$= Al_2Si_4O_{10}(OH)_2(\text{pyrophyllite}) + H_2O(\text{gas}) \qquad (B)$$

However, the reversed observations of Thompson (1970) lie well outside the 2 sigma limits. Figure 7 shows the calculated Gibbs

Figure 6. Error (observed value - calculated value)/precision as a function of temperature for the reaction: Kaolinite + 2 Quartz = Pyrophyllite + Steam. The open triangles were calculated from the silicic acid solubilities of Hemley and others (1980). The connected solid squares represent the brackets of Thompson (1970). The dashed lines represent two times the precision stated by the authors or two times the width of the Gibbs energy bracket, whichever is appropriate.

Kaolinite + 2 Quartz = Pyrophyllite + Steam



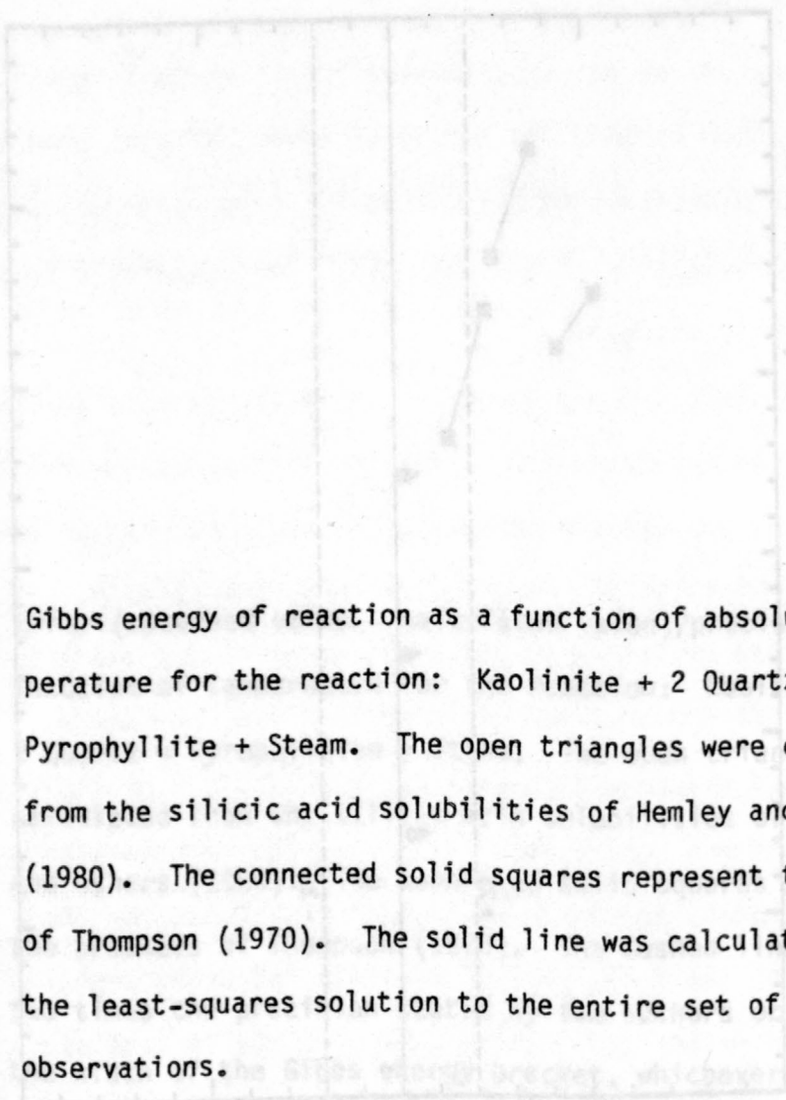


Figure 7. Gibbs energy of reaction as a function of absolute temperature for the reaction: Kaolinite + 2 Quartz = Pyrophyllite + Steam. The open triangles were calculated from the silicic acid solubilities of Hemley and others (1980). The connected solid squares represent the brackets of Thompson (1970). The solid line was calculated from the least-squares solution to the entire set of experimental observations.

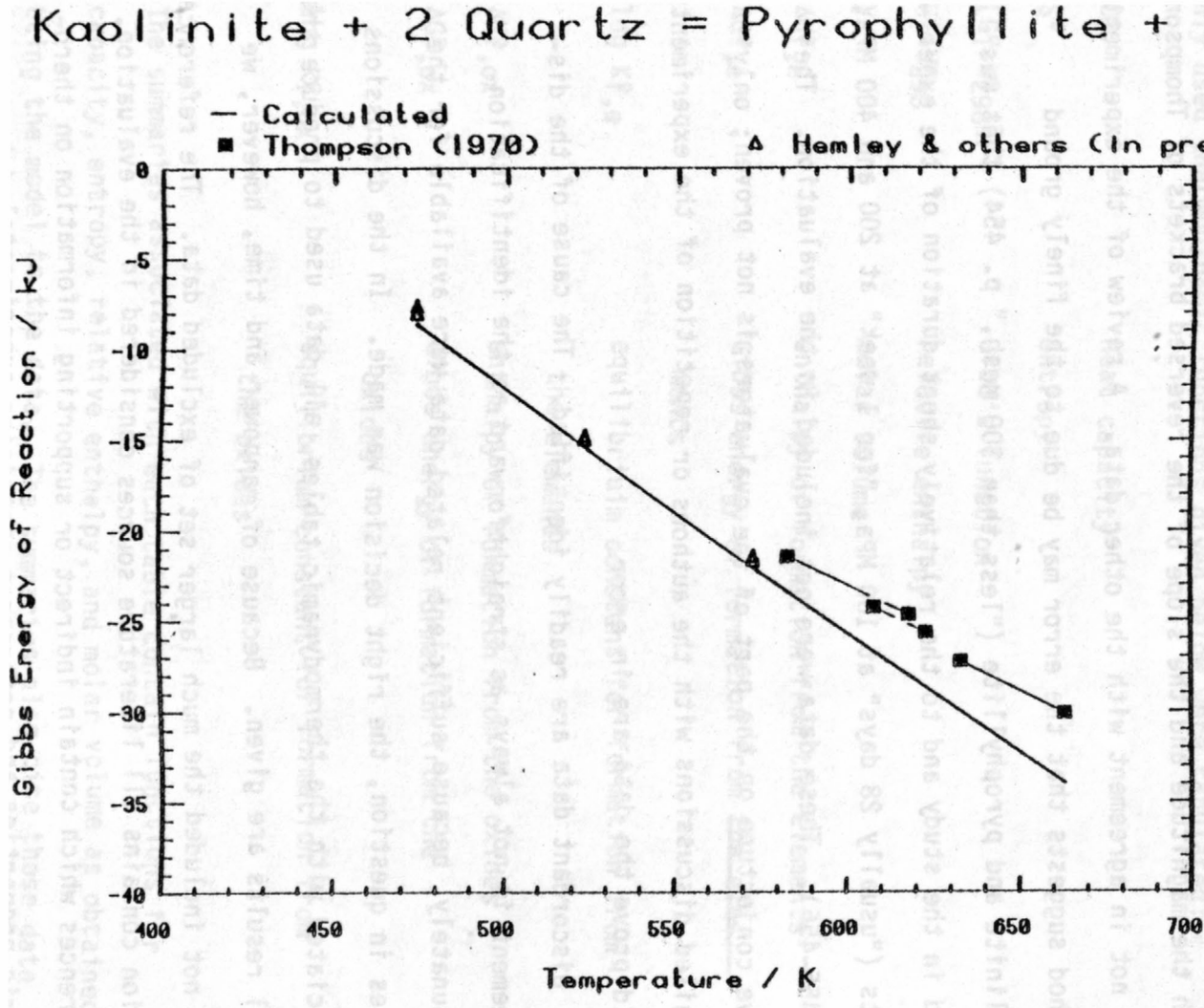


Figure 7, Robinson and others

energy for reaction B and the experimental data cited on figure 6. As expected, the data of Hemley and coworkers lie near the calculated values. Because the calculated line also reflects the other data in the problem, particularly entropies and other phase equilibria, we conclude that data of Hemley and coworkers are consistent. However, both the magnitude and the slope of the reversed brackets of Thompson are not in agreement with the other data. A review of the experimental method suggests that the error may be due to the finely ground kaolinite and pyrophyllite ("less than 300 mesh," p. 454) that was used in the study and to the relatively short duration of the experiments ("usually 28 days" at 100 MPa, "for 1 week" at 200 and 400 MPa, p. 455-456). These data were not included in the evaluation. The above conjecture on the part of the evaluators is not proven; only detailed discussions with the authors or repetition of the experiments could prove the data are in error.

Discordant data are readily identified. The cause of the disagreement is not always as straightforward as the identification. Fortunately, because sufficient related data were available for the phases in question, the right decision was made. In the discussions associated with the thermodynamic tables, all data used to produce the final results are given. Because of manpower and time, however, we have not included the much larger set of excluded data. The reference section contains all literature sources considered in the evaluation. References which contain indirect or supporting information on therodynamic properties and references containing experimental data considered, but excluded from the evaluation, are marked with an asterisk (*) at the beginning of the citation.

1.3.3.6. Preparation of tables and summaries

Tables of thermodynamic data at 101.325 kPa between 273.15 K and 1800 K were prepared from the functions in the fitted model. The commonly used thermodynamic functions given below were tabulated:

C_p°	heat capacity
S°	entropy
$[G_T^\circ - H_{298}^\circ]/T$	Gibb's function
$H_T^\circ - H_{298}^\circ$	relative enthalpy
V	molar volume
$\Delta H_{f,e}^\circ$	enthalpy of formation from the elements
$\Delta G_{f,e}^\circ$	Gibbs energy of formation from the elements
$\log K_{f,e}^\circ$	equilibriuim constant for formation from the elements
$\Delta H_{f,ox}^\circ$	enthalpy of formation from the oxides
$\Delta G_{f,ox}^\circ$	Gibbs energy of formation from the oxides
$\log K_{f,ox}^\circ$	equilibrium constant for formation from the oxides

The summaries associated with each table contain functions for heat capacity, entropy, relative enthalpy, and molar volume as obtained in fitting the model to the data. The summaries also cite those data used in the final evaluation that were directly pertinent to determine the properties of the phase in question. In the interest of saving manpower for more evaluations, data that were considered and rejected

are not tabulated.

1.3.3.7. Confidence limits

All evaluations must start with some base that is accepted without question. In this effort, the properties of the elements and the oxides cited in Appendix section 1.5.4 were used without question. The properties for the evaluated phases are determined relative to those reference values. In the course of the evaluation, we found no inconsistency of sufficient magnitude that would require us to consider reevaluating any of that reference base. This does not mean that the tabulated values are without error. For example, the uncertainty for the entropy at 298.15 K for Ca or CaO is about 1 percent (CODATA Task Group, 1978).

In preparing the tabulations, the 2-sigma confidence limits were given for the 298.15 K isotherm and for every isotherm that is a multiple of 250 K. These limits reflect only the variation in the final set of data on the chemical system. They do not include confidence limits on the reference data in Appendix section 1.5.4. For this reason the confidence limits for formation from the elements is omitted. If such a time arises when manpower is abundant or when other data centers adopt similar evaluation procedures, the imprecision in the reference base will be included in the tables.

1.3.3.8. Results

The Appendix, section 1.5, contains the thermochemical properties of phases of interest in exploring possible chemical reactions in basalt systems. These data, as tabulated, are consistent with the

recommendations of the CODATA Task Group (1978). In general, we used the same reference base as Robie and others (1979) and as used in preparing the JANAF Thermochemical Tables (Stull and Prophet, 1971) and the JANAF thermochemical data[a].

The arrangement of the compounds is alphabetical using the commonly accepted chemical formula for the phase. Sections 1.5.1 and 1.5.2 contain the index arranged by chemical formula and by mineral name, respectively.

[a]JANAF Thermochemical Tables, looseleaf pages for 1979 issued by Dow Chemical Company, 1707 Building, Midland, Michigan.

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1.5. Appendix - Thermodynamic Tables and Summaries

The refined thermodynamic properties (thermophysical, thermochemical, and volumetric) for the chemical compounds considered in this study are given in section 1.5.4 below. Sections 1.5.1 and 1.5.2 give the arrangement by chemical formula and the cross index for the minerals, respectively.

Section 1.5.3 gives algebraic and thermodynamic functions that were followed in this study. The summaries of data that were considered in this study, special comments appropriate for each phase, and the constants as would be used in equations in section 1.5.3 are given in section 1.5.5.

1.5.1. Chemical Index to Tables and Summaries

The compounds for which data are given in sections 1.5.4 and 1.5.5 are arranged alphabetically by the commonly accepted formula. The data in table 10 give the table numbers and pages on which the reader will find the needed properties.

1.5.2. Mineral Index to Tables and Summaries

The data, in table 11, are supplied as a convenient cross-index of mineral names, formulas, and property tables.

Table 10. Chemical index to tables and summaries.

Chemical formula (in order of arrangement)	Mineral name	Properties			Summaries Constants (page number)	
		Thermophysical	Thermochemical (table number)	Volumetric		
Al (crystal, liquid)	---	12	13	-	287	414,419
AlOOH	boehmite	14,16	15,17	146	287	414,419
AlOOH	diaspore	14,18	15,19	147	290	414,419
$Al(OH)_3$	gibbsite	20	21	148	293	414,419
Al_2O_3	corundum	22	23	149	296	414,419
Al_2SiO_5	andalusite	24,26	25,27	150	296	414,419
Al_2SiO_5	kyanite	24,28	25,29	151	300	414,419
Al_2SiO_5	sillimanite	24,30	25,31	152	303	414,419
$Al_2Si_2O_5(OH)_4$	kaolinite	32	33	153	306	414,419
$Al_2Si_2O_5(OH)_4$	dickite	34	35	154	306	414,419
$Al_2Si_2O_5(OH)_4$	halloysite	36	37	155	306	414,419
$Al_2Si_4O_{10}(OH)_2$	pyrophyllite	38	39	156	313	414,419
C	graphite	40	41	-	313	414,419
CO (ideal gas)	---	42	43	-	313	414,419
CO_2 (ideal gas)	---	44	45	-	313	415,420
Ca (crystal, liquid, ideal gas)	---	46	47	-	316	415,420
$CaAl_2SiO_6$	Ca-Al clinopyroxene	48	49	157	316	415,420
$CaAl_2Si_2O_8$	anorthite	50	51	158	316	415,420
$CaAl_4Si_2O_{10}(OH)_2$	margarite	52	53	159	323	415,420
$CaCO_3$	calcite	54	55	160	323	415,420
$CaCO_3$	aragonite	56	57	161	328	415,420
CaO	lime	58	59	162	328	415,420
$CaSiO_3$	wollastonite	60,62	61,63	163	332	415,420
$CaSiO_3$	cyclowollastonite	60,64	61,65	164	332	415,420

Table 10. Continued

Chemical formula (in order of arrangement)	Mineral name	Properties: Thermophysical	Thermochemical (table number)	Volumetric	Summaries (page number)	Constants (page number)
$Ca_2Al_2SiO_6(OH)_2$	bicchulite	66	67	165	338	415,420
$Ca_2Al_2SiO_7$	gehlenite	68	69	166	338	415,420
$Ca_2Al_2Si_3O_{10}(OH)_2$	prehnite	70	71	167	343	416,421
$Ca_2Al_3Si_3O_{12}(OH)$	zoisite	72	73	168	343	416,421
Ca_2SiO_4 (alpha)	---	74,76	75,77	169	354	416,421
Ca_2SiO_4 (alpha-prime)	bredigite	74,78	75,79	170	354	416,421
Ca_2SiO_4 (gamma)	Ca olivine	74,80	75,81	171	354	416,421
Ca_2SiO_4 (beta)	larnite	74,82	75,83	172	354	416,421
$Ca_3Al_2Si_3O_{12}$	grossular	84	85	173	356	416,421
Ca_3SiO_5	hatrurite	86	87	174	356	416,421
$Ca_3Si_2O_7$	rankinite	88	89	175	362	416,421
$Ca_4Al_6Si_6O_{24}(CO_3)$	melonite	90	91	176	362	416,421
Fe (alpha, alpha-prime, gamma)	---	92	93	-	362	416,421
$Fe_{.947}O$	wustite	94	95	177	367	416,421
$FeSiO_3$	ferrosilite	96	97	178	367	416,421
Fe_2O_3	hematite	98	99	179	373	417,422
Fe_2SiO_4	fayalite	100	101	180	376	417,422
Fe_3O_4	magnetite	102	103	181	379	417,422
H_2 (ideal gas)	---	104	105	-	379	417,422
H_2O (liquid)	water	106,108	107,109	182	382	417,422
H_2O (ideal gas)	---	106.110	107,111	-	382	417,422
H_2O (real gas)	---	-	-	182	382	417,422
H_4SiO_4, silicic acid	---	-	-	-	382	---

Table 10. Continued

Chemical formula (in order of arrangement)	Mineral name	Properties			Summaries (page number)	Constants (page number)
		Thermophysical	Thermochemical (table number)	Volumetric		
Mg	---	112	113	-	383	417,422
$MgCO_3$	magnesite	114	115	183	383	417,422
MgO	periclase	116	117	184	386	417,422
$Mg(OH)_2$	brucite	118	119	185	386	417,422
$MgSiO_3$	clinoenstatite	120,122	121,123	186	386	417,422
$MgSiO_3$	enstatite	120,124	121,125	187	386	418,423
$MgSiO_3$	protoenstatite	120,126	121,127	188	386	418,423
Mg_2SiO_4	forsterite	128	129	189	396	418,423
$Mg_3Si_2O_5(OH)_4$	chrysotile	130	131	190	396	418,423
$Mg_3Si_4O_{10}(OH)_2$	talc	132	133	191	396	418,423
$Mg_7Si_8O_{22}(OH)_2$	anthophyllite	134	135	192	396	418,423
$Mg_{48}Si_{34}O_{85}(OH)_{62}$	antigorite	136	137	193	407	418,423
O_2 (ideal gas)	---	138	139	-	407	418,423
Si (crystal, liquid)	---	140	141	-	407	418,423
SiO_2	quartz	142	143	194	410	418,423
SiO_2	cristobalite	144	145	195	410	418,423

Table 11. Mineral index to tables and summaries.

Mineral name	Chemical formula	Properties			Summaries (page number)	Constants (page number)
		Thermophysical	Thermochemical (table number)	Volumetric		
andalusite	Al_2SiO_5	24,26	25,27	150	296	414,419
anorthite	$CaAl_2Si_2O_8$	50	51	158	316	415,420
anthophyllite	$Mg_7Si_8O_{22}(OH)_2$	134	135	192	396	418,423
antigorite	$Mg_{48}Si_{34}O_{85}(OH)_{62}$	136	137	193	407	418,423
aragonite	$CaCO_3$	56	57	161	328	415,420
bicchulite	$Ca_2Al_2SiO_6(OH)_2$	66	67	165	338	415,420
boehmite	AlOOH	14,16	15,17	146	287	414,419
bredigite	Ca_2SiO_4 (alpha-prime)	74,78	75,79	170	354	416,421
brucite	$Mg(OH)_2$	118	119	185	386	417,422
Ca olivine	Ca_2SiO_4 (gamma)	74,80	75,81	171	354	416,421
Ca-Al clinopyroxene	$CaAl_2SiO_6$	48	49	157	316	415,420
calcite	$CaCO_3$	54	55	160	323	415,420
chrysotile	$Mg_3Si_2O_5(OH)_4$	130	131	190	396	418,423
clay minerals	See dickite, halloysite, kaolinite, pyrophyllite.					
clinoenstatite	$MgSiO_3$	120,122	121,123	186	386	417,422
corundum	Al_2O_3	22	23	149	296	414,419
cristobalite	SiO_2	144	145	195	410	418,423
cyclowollastonite	$CaSiO_3$	60,64	61,65	164	332	415,420
diaspore	AlOOH	14,18	15,19	147	290	414,419
dickite	$Al_2Si_2O_5(OH)_4$	34	35	154	306	414,419
enstatite	$MgSiO_3$	120,124	121,125	187	386	418,423
epidote group	See zoisite					
fayalite	Fe_2SiO_4	100	101	180	387	417,422

Table 11. Continued

Mineral name	Chemical formula	Properties			Summaries Constants (page number)	
		Thermophysical	Thermochemical (table number)	Volumetric		
feldspar group	See anorthite					
ferrosilite	$FeSiO_3$	96	97	178	367	416,421
forsterite	Mg_2SiO_4	128	129	189	396	418,423
garnet group	See grossular					
gehlenite	$Ca_2Al_2SiO_7$	68	69	166	338	415,420
gibbsite	$Al(OH)_3$	20	21	148	293	414,419
graphite	C	40	41	-	313	414,419
grossular	$Ca_3Al_2Si_3O_{12}$	84	85	173	356	416,421
halloysite	$Al_2Si_2O_5(OH)_4$	36	37	155	306	414,419
hatrurite	Ca_3SiO_5	86	87	174	356	416,421
hematite	Fe_2O_3	98	99	179	373	417,422
kaolinite	$Al_2Si_2O_5(OH)_4$	32	33	153	306	414,419
kyanite	Al_2SiO_5	24,28	25,29	151	300	414,419
larnite	Ca_2SiO_4 (beta)	74,82	75,83	172	354	416,421
lime	CaO	58	59	162	328	415,420
magnesite	$MgCO_3$	114	115	183	383	417,422
magnetite	Fe_3O_4	102	103	181	379	417,422
margarite	$CaAl_4Si_2O_{10}(OH)_2$	52	53	159	323	415,420
melonite	$Ca_4Al_6Si_6O_{24}(CO_3)$	90	91	176	362	416,421
melilite group	See gehlenite, rankinite					
olivine group	See Ca olivine, fayalite, forsterite					
periclase	MgO	116	117	184	386	417,422

Table 11. Continued

Mineral name	Chemical formula	Properties			Summaries (page number)	Constants (page number)
		Thermophysical	Thermochemical (table number)	Volumetric		
prehnite	$Ca_2Al_2Si_3O_{10}(OH)_2$	70	71	167	343	416,421
protoenstatite	$MgSiO_3$	120,126	121,127	188	386	418,423
"pseudowollastonite"	See cyclowollastonite					
pyrophyllite	$Al_2Si_4O_{10}(OH)_2$	38	39	156	313	414,419
pyroxene group	See Ca-Al clinopyroxene, clinoenstatite, enstatite, protoenstatite, ferrosilite, pyroxenoids					
pyroxenoids	See wollastonite, cyclowollastonite					
quartz	SiO_2	142	143	194	410	418,423
rankinite	$Ca_3Si_2O_7$	88	89	175	362	416,421
serpentine group	See antigorite, chrysotile					
sillimanite	Al_2SiO_5	24,30	25,31	152	303	414,419
talc	$Mg_3Si_4O_{10}(OH)_2$	132	133	191	396	418,423
water	H_2O (liquid)	106,108	107,109	182	382	417,422
wollastonite	$CaSiO_3$	60,62	61,63	163	332	415,420
wustite	$Fe_{.947}O$	94	95	177	367	416,421
zoisite	$Ca_2Al_3Si_3O_{12}(OH)$	72	73	168	343	416,421

1.5.3. Functions Describing Thermophysical Properties as a Function of Pressure and Temperature

General Thermodynamic Relationships

Thermodynamic theory provides the following exact functional relations among heat capacity (C_{p_r}) at a reference pressure P_r, volume (V), entropy (S), enthalpy (H), free energy (G), equilibrium constant (K), and electrochemical potential (E):

$$C_{p,i} - C_{p_r,i} = -\int_{P_r}^{P} T\,(\partial^2 V_i / \partial T_2)\,dP \tag{16}$$

$$S_i = S_0 + \int_0^T \frac{C_{p_r,i}}{T}\,dT - \int_{P_r}^{P} \left(\frac{\partial V_i}{\partial T}\right)_p dP \tag{17}$$

$$H_i = H_0 + \int_0^T C_{p_r,i}\,dT + \int_{P_r}^{P} \left(V_i - T\left(\frac{\partial V_i}{\partial T}\right)_p\right) dP \tag{18}$$

$$G_i = H_i - T\,S_i \tag{19}$$

$$-RT \ln K = \sum_{i=1}^{j} N_i\,G_i \tag{20}$$

$$-nFE = \sum_{i=1}^{j} N_i\,G_i \tag{21}$$

where T is thermodynamic temperature (Kelvin), R and F are the ideal gas constant and Faraday constant, respectively. The term j is the number of species in the reaction, and N_i is the stoichiometric coefficient, positive for products and negative for each reactant (i). The term n is the

number of electrons involved in the reaction. From these, it follows that an empirical relation which describes heat capacity ($C_{p_r,i}$) as a function of temperature and volume (V_i) as a function of temperature and pressure will generate the mathematical description of the other thermodynamic properties.

Formulae Describing Thermodynamic Properties

$$C_{p_r,i} = \frac{a_{1,i}}{T^2} + \frac{a_{3,i}}{T^{1/2}} + a_{5,i} + 2a_{6,i}\, T + a_{7,i}\, T^2 \tag{22}$$

$$V_i = b_{1,i} + b_{2,i}\, T + b_{3,i}\, \exp(-T/300) + b_{4,i}\, P + b_{5,i}\, \exp(-P/35000) \tag{23}$$

$$C_{p,i} - C_{p_r,i} = \frac{-b_{3,i}}{90000}\, T \exp(-T/300)(P - P_r) \tag{24}$$

$$H_i = \frac{-a_{1,i}}{T} + a_{2,i} + 2\, a_{3,i} \sqrt{T} + a_{5,i}\, T + a_{6,i}\, T^2 + a_{7,i} \frac{T^3}{3} +$$

$$b_{1,i}\, (P - P_r) + b_{3,i}\, (1 + \frac{T}{300})\, (\exp(-T/300))\, (P - P_r) +$$

$$\frac{b_{4,i}}{2}\, (P^2 - P_r^2) - (35000)\, b_{5,i}\, \{\exp(-P/35000) -$$

$$\exp(-P_r/35000)\} \tag{25}$$

$$S_i = \frac{-a_{1,i}}{2T^2} - \frac{2a_{3,i}}{\sqrt{T}} + a_{4,i} + a_{5i} \ln T + 2\, a_{6,i}\, T + a_{7,i} \frac{T^2}{2} -$$

$$b_{2,i}\, (P - P_r) + (\frac{b_{3,i}}{300})\, (P - P_r) \exp(-T/300) \tag{26}$$

$$G_i = -\frac{a_{1,i}}{2T} + a_{2,i} - 4\,a_{3,i}\sqrt{T} - a_{4,i}\,T + a_{5,i}\,(T - T\ln T) -$$

$$a_{6,i}\,T^2 - a_{7,i}\,\frac{T^3}{6} + b_{1,i}\,(P - P_r) + b_{2,i}\,T\,(P - P_r) +$$

$$b_{3,i}\,(P - P_r)\exp(-T/300) + \frac{b_{4,i}}{2}\,(P^2 - P_r^2) -$$

$$(35000)\,b_{5,i}\,\{\exp(-P/35000) - \exp(-P_r/35000)\} \qquad (27)$$

1.5.4 Tables of Mineral Thermodynamic and Thermophysical Properties at 101.325 kPa (1 atm)

Page 128 follows

Table 12. Thermophysical values for stable phases of the element aluminum (Al) at 1.01325 bars (1 atm). The sources of data are given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
		aluminum (crystal)			
200.	21.513	19.138	-2273.	-30.505	---
250.	23.308	24.153	-1148.	-28.745	---
(2 sigma)	---	---	---	---	---
273.15	23.844	26.241	-602.	-28.445	---
298.15	24.307	28.350	0.	-28.350	---
(2 sigma)	---	---	---	---	---
300.	24.338	28.500	45.	-28.351	---
350.	25.049	32.308	1281.	-28.650	---
400.	25.625	35.691	2548.	-29.322	---
450.	26.157	38.741	3842.	-30.202	---
500.	26.692	41.524	5163.	-31.197	---
(2 sigma)	---	---	---	---	---
550.	27.255	44.094	6512.	-32.254	---
600.	27.863	46.491	7890.	-33.342	---
650.	28.525	48.747	9299.	-34.441	---
700.	29.249	50.887	10743.	-35.540	---
750.	30.039	52.932	12225.	-36.632	---
(2 sigma)	---	---	---	---	---
800.	30.898	54.898	13748.	-37.712	---
850.	31.828	56.798	15316.	-38.779	---
900.	32.831	58.645	16932.	-39.832	---
933.25	33.539	59.849	18036.	-40.524	---
		aluminum (liquid)			
933.25	31.756	71.413	28828.	-40.524	---
950.	31.756	71.978	29360.	-41.073	---
1000.	31.756	73.607	30948.	-42.660	---
(2 sigma)	---	---	---	---	---
1050.	31.756	75.157	32535.	-44.170	---
1100.	31.756	76.634	34123.	-45.613	---
1150.	31.756	78.045	35711.	-46.992	---
1200.	31.756	79.397	37299.	-48.315	---
1250.	31.756	80.693	38887.	-49.584	---
(2 sigma)	---	---	---	---	---
1300.	31.756	81.939	40474.	-50.805	---
1350.	31.756	83.137	42062.	-51.980	---
1400.	31.756	84.292	43650.	-53.114	---
1450.	31.756	85.407	45238.	-54.208	---
1500.	31.756	86.483	46826.	-55.266	---
(2 sigma)	---	---	---	---	---
1550.	31.756	87.525	48414.	-56.290	---
1600.	31.756	88.533	50001.	-57.282	---
1650.	31.756	89.510	51589.	-58.244	---
1700.	31.756	90.458	53177.	-59.177	---
1750.	31.756	91.379	54765.	-60.084	---
(2 sigma)	---	---	---	---	---
1800.	31.756	92.273	56353.	-60.966	---
(2 sigma)	---	---	---	---	---

Table 13. Thermochemical properties of stable phases of the element aluminum (Al) at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
			aluminum (crystal)			
200.	0.	0.	0.	---	---	---
250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
273.15	0.	0.	0.	---	---	---
298.15	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
300.	0.	0.	0.	---	---	---
350.	0.	0.	0.	---	---	---
400.	0.	0.	0.	---	---	---
450.	0.	0.	0.	---	---	---
500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
550.	0.	0.	0.	---	---	---
600.	0.	0.	0.	---	---	---
650.	0.	0.	0.	---	---	---
700.	0.	0.	0.	---	---	---
750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
800.	0.	0.	0.	---	---	---
850.	0.	0.	0.	---	---	---
900.	0.	0.	0.	---	---	---
933.25	0.	0.	0.	---	---	---
			aluminum (liquid)			
933.25	0.	0.	0.	---	---	---
950.	0.	0.	0.	---	---	---
1000.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1050.	0.	0.	0.	---	---	---
1100.	0.	0.	0.	---	---	---
1150.	0.	0.	0.	---	---	---
1200.	0.	0.	0.	---	---	---
1250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1300.	0.	0.	0.	---	---	---
1350.	0.	0.	0.	---	---	---
1400.	0.	0.	0.	---	---	---
1450.	0.	0.	0.	---	---	---
1500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1550.	0.	0.	0.	---	---	---
1600.	0.	0.	0.	---	---	---
1650.	0.	0.	0.	---	---	---
1700.	0.	0.	0.	---	---	---
1750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1800.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---

Table 14. Thermophysical values for stable phases with the composition AlOOH at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
		diaspore			
200.	34.372	17.801	-4373.	-39.664	17.6435
250.	45.103	26.675	-2374.	-36.172	17.7030
(2 sigma)	0.108	0.099	5.	0.097	0.1664
273.15	49.230	30.852	-1281.	-35.544	17.7305
298.15	53.214	35.339	0.	-35.339	17.7602
(2 sigma)	0.114	0.097	0.	0.097	0.1333
300.	53.491	35.669	99.	-35.340	17.7624
350.	60.222	44.438	2947.	-36.017	17.8219
400.	65.750	52.852	6101.	-37.600	17.8813
450.	70.379	60.871	9507.	-39.744	17.9407
500.	74.319	68.496	13127.	-42.241	18.0002
(2 sigma)	0.442	0.155	51.	0.099	0.3905
550.	77.718	75.742	16930.	-44.960	18.0596
582.7	79.701	80.291	19505.	-46.817	18.0985
		boehmite			
582.7	101.862	104.718	33739.	-46.817	20.3905
600.	103.356	107.720	35514.	-48.530	20.4425
650.	107.402	116.156	40785.	-53.410	20.5929
700.	111.098	124.252	46249.	-58.183	20.7432
750.	114.497	132.035	51890.	-62.849	20.8935
(2 sigma)	0.594	0.445	511.	0.605	0.5907
800.	117.645	139.526	57694.	-67.408	21.0438
850.	120.576	146.747	63650.	-71.864	21.1942
900.	123.319	153.717	69749.	-76.219	21.3445
950.	125.899	160.455	75980.	-80.476	21.4948
1000.	128.336	166.975	82336.	-84.639	21.6452
(2 sigma)	0.755	0.569	578.	0.492	0.9140
1050.	130.644	173.293	88811.	-88.711	21.7955
1100.	132.840	179.422	95399.	-92.696	21.9458
1150.	134.935	185.373	102093.	-96.596	22.0961
1200.	136.938	191.159	108891.	-100.416	22.2465
1250.	138.860	196.788	115786.	-104.159	22.3968
(2 sigma)	1.226	0.675	686.	0.457	1.2381

Table 15. Thermochemical properties of stable phases with the composition AlOOH at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements: columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
			diaspore			
200.	-997816.	-946920.	247.310	---	---	---
250.	-999077.	-934042.	195.157	---	---	---
(2 sigma)	---	---	---	---	---	---
273.15	-999533.	-927998.	177.462	-18555.	-12290.	2.350
298.15	-999944.	-921432.	161.431	-19171.	-11689.	2.048
(2 sigma)	---	---	---	406.	403.	0.071
300.	-999971.	-920945.	160.351	-19215.	-11643.	2.027
350.	-1000563.	-907723.	135.470	-20351.	-10289.	1.536
400.	-1000910.	-894434.	116.801	-41263.	-7330.	0.957
450.	-1001058.	-881114.	102.277	-41179.	-3092.	0.359
500.	-1001042.	-867786.	90.657	-41019.	1132.	-0.118
(2 sigma)	---	---	---	414.	401.	0.042
550.	-1000894.	-854467.	81.150	-40791.	5336.	-0.507
582.7	-1000738.	-845767.	75.817	-40609.	8073.	-0.724
			boehmite			
582.7	-986503.	-845767.	75.817	-26375.	8073.	-0.724
600.	-986017.	-841595.	73.267	-25881.	9088.	-0.791
650.	-984506.	-829620.	66.669	-24370.	11942.	-0.960
700.	-982857.	-817767.	61.022	-22741.	14675.	-1.095
750.	-981090.	-806036.	56.137	-21001.	17287.	-1.204
(2 sigma)	---	---	---	511.	453.	0.032
800.	-979219.	-794426.	51.871	-19158.	19780.	-1.292
850.	-977261.	-782936.	48.113	-17216.	22155.	-1.361
900.	-975228.	-771564.	44.780	-15182.	24413.	-1.417
950.	-983761.	-759982.	41.787	-13059.	26555.	-1.460
1000.	-981477.	-748263.	39.085	-10852.	28583.	-1.493
(2 sigma)	---	---	---	578.	492.	0.026
1050.	-979091.	-736661.	36.647	-8565.	30499.	-1.517
1100.	-976608.	-725174.	34.436	-6200.	32304.	-1.534
1150.	-974034.	-713803.	32.422	-3762.	34000.	-1.544
1200.	-971372.	-702545.	30.581	-1253.	35588.	-1.549
1250.	-968627.	-691400.	28.892	1324.	37071.	-1.549
(2 sigma)	---	---	---	686.	571.	0.024

Table 16. Thermophysical values for boehmite, AlOOH, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	42.915	26.850	-5383.	-53.762	19.2399
250.	55.388	37.807	-2916.	-49.470	19.3902
(2 sigma)	0.081	0.273	4.	0.273	0.0920
273.150	60.435	42.936	-1574.	-48.699	19.4598
298.150	65.427	48.447	0.	-48.447	19.5350
(2 sigma)	0.118	0.273	0.	0.273	0.0675
300.	65.779	48.853	121.	-48.448	19.5406
350.	74.487	59.666	3634.	-49.282	19.6909
400.	81.897	70.108	7549.	-51.237	19.8412
450.	88.299	80.133	11807.	-53.895	19.9915
500.	93.910	89.733	16365.	-57.002	20.1419
(2 sigma)	0.459	0.307	59.	0.274	0.2707
550.	98.889	98.921	21188.	-60.398	20.2922
600.	103.356	107.720	26246.	-63.978	20.4425
650.	107.402	116.156	31516.	-67.669	20.5929
700.	111.098	124.252	36980.	-71.424	20.7432
750.	114.497	132.035	42621.	-75.207	20.8935
(2 sigma)	0.594	0.445	190.	0.290	0.5907
800.	117.645	139.526	48426.	-78.994	21.0438
850.	120.576	146.747	54382.	-82.768	21.1942
900.	123.319	153.717	60480.	-86.517	21.3445
950.	125.899	160.455	66711.	-90.233	21.4948
1000.	128.336	166.975	73068.	-93.908	21.6452
(2 sigma)	0.755	0.569	327.	0.327	0.9140
1050.	130.644	173.293	79543.	-97.538	21.7955
1100.	132.840	179.422	86130.	-101.122	21.9458
1150.	134.935	185.373	92825.	-104.656	22.0961
1200.	136.938	191.159	99622.	-108.140	22.2465
1250.	138.860	196.788	106517.	-111.574	22.3968
(2 sigma)	1.226	0.675	493.	0.370	1.2381

Table 17. Thermochemical properties of boehmite, AlOOH, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-989557.	-940471.	245.626	---	---	---
250.	-990350.	-928098.	193.915	---	---	---
(2 sigma)	---	---	---	---	---	---
273.150	-990557.	-922323.	176.376	-9579.	-6615.	1.265
298.150	-990675.	-916072.	160.492	-9902.	-6329.	1.109
(2 sigma)	---	---	---	468.	450.	0.079
300.	-990680.	-915609.	159.422	-9923.	-6306.	1.098
350.	-990608.	-903098.	134.780	-10395.	-5664.	0.845
400.	-990194.	-890621.	116.303	-30547.	-3516.	0.459
450.	-989489.	-878213.	101.940	-29611.	-191.	0.022
500.	-988536.	-865898.	90.460	-28512.	3020.	-0.315
(2 sigma)	---	---	---	474.	446.	0.047
550.	-987368.	-853690.	81.077	-27265.	6114.	-0.581
600.	-986017.	-841595.	73.267	-25881.	9088.	-0.791
650.	-984506.	-829620.	66.669	-24370.	11942.	-0.960
700.	-982857.	-817767.	61.022	-22741.	14675.	-1.095
750.	-981090.	-806036.	56.137	-21001.	17287.	-1.204
(2 sigma)	---	---	---	511.	453.	0.032
800.	-979219.	-794426.	51.871	-19158.	19780.	-1.292
850.	-977261.	-782936.	48.113	-17216.	22155.	-1.361
900.	-975228.	-771564.	44.780	-15182.	24413.	-1.417
950.	-983761.	-759982.	41.787	-13059.	26555.	-1.460
1000.	-981477.	-748263.	39.085	-10852.	28583.	-1.493
(2 sigma)	---	---	---	578.	492.	0.026
1050.	-979091.	-736661.	36.647	-8565.	30499.	-1.517
1100.	-976608.	-725174.	34.436	-6200.	32304.	-1.534
1150.	-974034.	-713803.	32.422	-3762.	34000.	-1.544
1200.	-971372.	-702545.	30.581	-1253.	35588.	-1.549
1250.	-968627.	-691400.	28.892	1324.	37071.	-1.549
(2 sigma)	---	---	---	686.	571.	0.024

Table 18. Thermophysical values for diaspore, AlOOH, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	34.372	17.801	-4373.	-39.664	17.6435
250.	45.103	26.675	-2374.	-36.172	17.7030
(2 sigma)	0.108	0.099	5.	0.097	0.1664
273.15	49.230	30.852	-1281.	-35.544	17.7305
298.15	53.214	35.339	0.	-35.339	17.7602
(2 sigma)	0.114	0.097	0.	0.097	0.1333
300.	53.491	35.669	99.	-35.340	17.7624
350.	60.222	44.438	2947.	-36.017	17.8219
400.	65.750	52.852	6101.	-37.600	17.8813
450.	70.379	60.871	9507.	-39.744	17.9407
500.	74.319	68.496	13127.	-42.241	18.0002
(2 sigma)	0.442	0.155	51.	0.099	0.3905
550.	77.718	75.742	16930.	-44.960	18.0596
600.	80.684	82.635	20892.	-47.815	18.1191
650.	83.297	89.198	24993.	-50.747	18.1785
700.	85.618	95.458	29217.	-53.719	18.2380
750.	87.693	101.437	33551.	-56.703	18.2974
(2 sigma)	0.722	0.355	191.	0.132	0.8449
800.	89.562	107.157	37983.	-59.679	18.3569
850.	91.253	112.638	42504.	-62.634	18.4163
900.	92.791	117.898	47106.	-65.559	18.4758
950.	94.195	122.954	51781.	-68.447	18.5352
1000.	95.483	127.818	56523.	-71.295	18.5946
(2 sigma)	1.105	0.561	386.	0.201	1.3083

Table 19. Thermochemical properties of diaspore, AlOOH, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-997816.	-946920.	247.310	---	---	---
250.	-999077.	-934042.	195.157	---	---	---
(2 sigma)	---	---	---	---	---	---
273.15	-999533.	-927998.	177.462	-18555.	-12290.	2.350
298.15	-999944.	-921432.	161.431	-19171.	-11689.	2.048
(2 sigma)	---	---	---	406.	403.	0.071
300.	-999971.	-920945.	160.351	-19215.	-11643.	2.027
350.	-1000563.	-907723.	135.470	-20351.	-10289.	1.536
400.	-1000910.	-894434.	116.801	-41263.	-7330.	0.957
450.	-1001058.	-881114.	102.277	-41179.	-3092.	0.359
500.	-1001042.	-867786.	90.657	-41019.	1132.	-0.118
(2 sigma)	---	---	---	414.	401.	0.042
550.	-1000894.	-854467.	81.150	-40791.	5336.	-0.507
600.	-1000639.	-841166.	73.230	-40503.	9518.	-0.829
650.	-1000298.	-827890.	66.530	-40162.	13673.	-1.099
700.	-999889.	-814643.	60.789	-39773.	17799.	-1.328
750.	-999429.	-801427.	55.816	-39341.	21897.	-1.525
(2 sigma)	---	---	---	463.	401.	0.028
800.	-998931.	-788243.	51.467	-38869.	25964.	-1.695
850.	-998408.	-775091.	47.631	-38363.	30001.	-1.844
900.	-997871.	-761970.	44.224	-37825.	34007.	-1.974
950.	-1007960.	-748555.	41.158	-37258.	37982.	-2.088
1000.	-1007290.	-734919.	38.388	-36665.	41927.	-2.190
(2 sigma)	---	---	---	579.	426.	0.022

Table 20. Thermophysical values for gibbsite, $Al(OH)_3$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	60.817	38.082	-7564.	-75.900	31.9033
250.	77.745	53.518	-4089.	-69.874	31.9301
(2 sigma)	0.091	0.361	5.	0.360	0.0774
273.15	84.744	60.712	-2207.	-68.793	31.9426
298.15	91.756	68.440	0.	-68.440	31.9560
(2 sigma)	0.151	0.360	0.	0.360	0.0772
300.	92.254	69.009	170.	-68.442	31.9570
350.	104.736	84.190	5102.	-69.612	31.9839
400.	115.626	98.903	10617.	-72.359	32.0107
450.	125.273	113.089	16644.	-76.102	32.0376
500.	133.936	126.744	23128.	-80.487	32.0645
(2 sigma)	0.837	0.435	102.	0.363	0.0814
550.	141.813	139.884	30025.	-85.294	32.0913
600.	149.049	152.538	37299.	-90.373	32.1182
650.	155.758	164.737	44921.	-95.627	32.1450
700.	162.026	176.511	52867.	-100.987	32.1719
750.	167.923	187.893	61117.	-106.403	32.1988
(2 sigma)	1.419	0.759	370.	0.402	0.0966
800.	173.504	198.910	69654.	-111.842	32.2256
850.	178.812	209.589	78463.	-117.280	32.2525
900.	183.884	219.955	87532.	-122.697	32.2794
950.	188.750	230.028	96848.	-128.082	32.3062
1000.	193.434	239.829	106404.	-133.426	32.3331
(2 sigma)	2.308	1.161	774.	0.501	0.1188

Table 21. Thermochemical properties of gibbsite, $Al(OH)_3$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-1291535.	-1201456.	313.788	---	---	---
250.	-1293406.	-1178707.	246.277	---	---	---
(2 sigma)	---	---	---	---	---	---
273.15	-1294065.	-1168055.	223.368	-26474.	-11074.	2.118
298.15	-1294633.	-1156496.	202.613	-28052.	-9593.	1.681
(2 sigma)	---	---	---	620.	630.	0.110
300.	-1294669.	-1155639.	201.214	-28164.	-9478.	1.650
350.	-1295369.	-1132404.	169.002	-30977.	-6136.	0.916
400.	-1295566.	-1109104.	144.834	-93054.	1936.	-0.253
450.	-1295318.	-1085807.	126.037	-92071.	13754.	-1.597
500.	-1294677.	-1062559.	111.005	-90793.	25447.	-2.658
(2 sigma)	---	---	---	629.	646.	0.068
550.	-1293685.	-1039393.	98.713	-89242.	36998.	-3.514
600.	-1292380.	-1016331.	88.479	-87440.	48396.	-4.213
650.	-1290792.	-993389.	79.830	-85405.	59635.	-4.792
700.	-1288949.	-970580.	72.425	-83151.	70709.	-5.276
750.	-1286872.	-947910.	66.018	-80691.	81614.	-5.684
(2 sigma)	---	---	---	722.	690.	0.048
800.	-1284584.	-925386.	60.421	-78035.	92349.	-6.030
850.	-1282102.	-903011.	55.492	-75192.	102912.	-6.324
900.	-1279441.	-880788.	51.120	-72171.	113302.	-6.576
950.	-1287246.	-858393.	47.198	-68978.	123520.	-6.792
1000.	-1284135.	-835901.	43.663	-65619.	133565.	-6.977
(2 sigma)	---	---	---	992.	798.	0.042

Table 22. Thermophysical values for corundum, Al_2O_3, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	50.491	24.844	-6509.	-57.386	25.5339
250.	67.336	38.033	-3538.	-52.183	25.5667
(2 sigma)	---	---	---	---	---
273.15	73.389	44.267	-1907.	-51.248	25.5819
298.15	79.030	50.943	0.	-50.943	25.5983
(2 sigma)	---	---	---	---	---
300.	79.416	51.433	147.	-50.945	25.5995
350.	88.490	64.388	4354.	-51.947	25.6323
400.	95.532	76.682	8962.	-54.278	25.6650
450.	101.132	88.270	13884.	-57.417	25.6978
500.	105.668	99.168	19057.	-61.053	25.7306
(2 sigma)	---	---	---	---	---
550.	109.397	109.420	24437.	-64.989	25.7634
600.	112.500	119.075	29987.	-69.098	25.7961
650.	115.108	128.186	35679.	-73.296	25.8289
700.	117.319	136.800	41491.	-77.527	25.8617
750.	119.209	144.960	47405.	-81.753	25.8945
(2 sigma)	---	---	---	---	---
800.	120.835	152.707	53407.	-85.948	25.9273
850.	122.244	160.076	59485.	-90.093	25.9600
900.	123.473	167.098	65629.	-94.178	25.9928
950.	124.552	173.804	71830.	-98.193	26.0256
1000.	125.506	180.217	78082.	-102.135	26.0584
(2 sigma)	---	---	---	---	---
1050.	126.356	186.362	84379.	-106.001	26.0911
1100.	127.118	192.258	90716.	-109.789	26.1239
1150.	127.809	197.924	97089.	-113.498	26.1567
1200.	128.439	203.377	103496.	-117.130	26.1895
1250.	129.021	208.632	109933.	-120.686	26.2222
(2 sigma)	---	---	---	---	---
1300.	129.563	213.703	116397.	-124.166	26.2550
1350.	130.073	218.602	122888.	-127.574	26.2878
1400.	130.559	223.341	129404.	-130.910	26.3206
1450.	131.026	227.931	135944.	-134.177	26.3533
1500.	131.481	232.381	142507.	-137.376	26.3861
(2 sigma)	---	---	---	---	---
1550.	131.928	236.699	149092.	-140.511	26.4189
1600.	132.372	240.895	155699.	-143.583	26.4517
1650.	132.815	244.975	162329.	-146.594	26.4844
1700.	133.262	248.947	168981.	-149.546	26.5172
1750.	133.717	252.816	175655.	-152.442	26.5500
(2 sigma)	---	---	---	---	---
1800.	134.180	256.589	182353.	-155.282	26.5828
(2 sigma)	---	---	---	---	---

Table 23. Thermochemical properties of corundum, Al_2O_3, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-1673409.	-1612703.	421.195	0.0	0.0	0.0
250.	-1674870.	-1597344.	333.746	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
273.15	-1675343.	-1590143.	304.084	0.0	0.0	0.0
298.15	-1675738.	-1582326.	277.217	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
300.	-1675763.	-1581747.	275.406	0.0	0.0	0.0
350.	-1676247.	-1566034.	233.718	0.0	0.0	0.0
400.	-1676430.	-1550274.	202.445	0.0	0.0	0.0
450.	-1676390.	-1534505.	178.121	0.0	0.0	0.0
500.	-1676186.	-1518749.	158.663	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
550.	-1675866.	-1503020.	142.745	0.0	0.0	0.0
600.	-1675467.	-1487324.	129.483	0.0	0.0	0.0
650.	-1675020.	-1471664.	118.264	0.0	0.0	0.0
700.	-1674551.	-1456038.	108.651	0.0	0.0	0.0
750.	-1674083.	-1440447.	100.322	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
800.	-1673635.	-1424886.	93.035	0.0	0.0	0.0
850.	-1673225.	-1409352.	86.608	0.0	0.0	0.0
900.	-1672869.	-1393840.	80.896	0.0	0.0	0.0
950.	-1693839.	-1377699.	75.751	0.0	0.0	0.0
1000.	-1693359.	-1361073.	71.095	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1050.	-1692852.	-1344471.	66.884	0.0	0.0	0.0
1100.	-1692323.	-1327894.	63.056	0.0	0.0	0.0
1150.	-1691774.	-1311341.	59.563	0.0	0.0	0.0
1200.	-1691207.	-1294812.	56.362	0.0	0.0	0.0
1250.	-1690624.	-1278308.	53.418	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1300.	-1690026.	-1261827.	50.701	0.0	0.0	0.0
1350.	-1689413.	-1245369.	48.186	0.0	0.0	0.0
1400.	-1688787.	-1228935.	45.852	0.0	0.0	0.0
1450.	-1688146.	-1212523.	43.680	0.0	0.0	0.0
1500.	-1687492.	-1196133.	41.653	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1550.	-1686823.	-1179765.	39.758	0.0	0.0	0.0
1600.	-1686139.	-1163420.	37.982	0.0	0.0	0.0
1650.	-1685439.	-1147095.	36.314	0.0	0.0	0.0
1700.	-1684723.	-1130793.	34.745	0.0	0.0	0.0
1750.	-1683988.	-1114511.	33.266	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1800.	-1683234.	-1098251.	31.870	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0

Table 24. Thermophysical values for stable phases with the composition Al_2SiO_5 at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
		kyanite			
200.	80.961	41.807	-10116.	-92.388	44.1175
250.	104.208	62.455	-5468.	-84.326	44.1618
(2 sigma)	0.145	0.303	6.	0.303	0.0306
273.15	113.385	72.091	-2947.	-82.881	44.1833
298.15	122.219	82.410	0.	-82.410	44.2071
(2 sigma)	0.121	0.302	0.	0.302	0.0229
300.	122.831	83.168	227.	-82.413	44.2089
350.	137.448	103.246	6748.	-83.965	44.2584
400.	148.930	122.380	13919.	-87.581	44.3098
408.450	150.616	125.511	15185.	-88.334	44.3187
		andalusite			
408.450	150.075	134.690	18934.	-88.334	51.6899
450.	156.958	149.568	25317.	-93.307	51.7443
500.	163.667	166.465	33339.	-99.787	51.8128
(2 sigma)	0.294	0.353	421.	0.653	0.0222
550.	169.038	182.326	41662.	-106.577	51.8841
600.	173.382	197.227	50226.	-113.517	51.9578
650.	176.937	211.250	58987.	-120.500	52.0335
700.	179.886	224.473	67910.	-127.459	52.1109
750.	182.375	236.971	76968.	-134.347	52.1898
(2 sigma)	0.313	0.377	433.	0.408	0.0230
800.	184.520	248.811	86141.	-141.135	52.2699
850.	186.413	260.056	95416.	-147.802	52.3511
900.	188.131	270.760	104780.	-154.338	52.4331
942.450	189.500	279.462	112795.	-159.779	52.5033
		sillimanite			
942.450	189.991	283.311	116423.	-159.779	50.4826
950.	190.273	284.828	117858.	-160.767	50.4892
1000.	192.164	294.636	127419.	-167.217	50.5332
(2 sigma)	0.452	0.368	391.	0.372	0.0109
1050.	194.126	304.059	137076.	-173.510	50.5777
1100.	196.204	313.137	146834.	-179.652	50.6225
1150.	198.433	321.907	156699.	-185.647	50.6676
1200.	200.847	330.403	166680.	-191.503	50.7130
1250.	203.472	338.654	176787.	-197.225	50.7586
(2 sigma)	0.892	0.380	409.	0.337	0.0170
1300.	206.334	346.689	187031.	-202.819	50.8044
1350.	209.453	354.534	197425.	-208.294	50.8503
1400.	212.848	362.212	207981.	-213.654	50.8964
1450.	216.535	369.745	218714.	-218.907	50.9425
1500.	220.529	377.152	229640.	-224.059	50.9888
(2 sigma)	2.830	0.474	609.	0.320	0.0303
1550.	224.842	384.452	240773.	-229.115	51.0351
1600.	229.488	391.663	252129.	-234.082	51.0816
1650.	234.475	398.800	263727.	-238.966	51.1280
1700.	239.813	405.879	275583.	-243.771	51.1746
1750.	245.511	412.912	287714.	-248.503	51.2211
(2 sigma)	6.160	1.001	1568.	0.321	0.0456
1800.	251.576	419.912	300140.	-253.168	51.2677
(2 sigma)	6.994	1.171	1882.	0.327	0.0488

Table 25. Thermochemical properties of stable phases with the composition Al_2SiO_5 at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
			kyanite			
200.	-2592988.	-2494666.	651.539	-9699.	-7887.	2.060
250.	-2595078.	-2469826.	516.041	-9834.	-7419.	1.550
(2 sigma)	---	---	---	520.	491.	0.103
273.15	-2595769.	-2458195.	470.082	-9891.	-7193.	1.375
298.15	-2596346.	-2445577.	428.455	-9937.	-6944.	1.217
(2 sigma)	---	---	---	520.	487.	0.085
300.	-2596382.	-2444641.	425.650	-9940.	-6925.	1.206
350.	-2597064.	-2419289.	361.059	-9986.	-6418.	0.958
400.	-2597272.	-2393874.	312.608	-9987.	-5908.	0.772
408.450	-2597269.	-2389577.	305.591	-9985.	-5822.	0.745
			andalusite			
408.450	-2593520.	-2389577.	305.591	-6236.	-5822.	0.745
450.	-2593410.	-2368835.	274.967	-6252.	-5779.	0.671
500.	-2593070.	-2343898.	244.865	-6303.	-5724.	0.598
(2 sigma)	---	---	---	504.	438.	0.046
550.	-2592568.	-2319004.	220.241	-6401.	-5662.	0.538
600.	-2591961.	-2294161.	199.724	-6558.	-5589.	0.487
650.	-2591291.	-2269371.	182.369	-6781.	-5499.	0.442
700.	-2590596.	-2244634.	167.497	-7077.	-5390.	0.402
750.	-2589901.	-2219947.	154.611	-7447.	-5257.	0.366
(2 sigma)	---	---	---	512.	429.	0.030
800.	-2589230.	-2195306.	143.339	-7892.	-5097.	0.333
850.	-2588602.	-2170705.	133.395	-9121.	-4902.	0.301
900.	-2588029.	-2146140.	124.559	-9286.	-4649.	0.270
942.450	-2608884.	-2124834.	117.767	-9425.	-4427.	0.245
			sillimanite			
942.450	-2605257.	-2124834.	117.767	-5798.	-4427.	0.245
950.	-2605150.	-2120986.	116.620	-5818.	-4416.	0.243
1000.	-2604413.	-2095523.	109.459	-5945.	-4339.	0.227
(2 sigma)	---	---	---	550.	489.	0.026
1050.	-2603620.	-2070097.	102.982	-6045.	-4256.	0.212
1100.	-2602765.	-2044711.	97.095	-6110.	-4169.	0.198
1150.	-2601836.	-2019366.	91.722	-6128.	-4080.	0.185
1200.	-2600825.	-1994062.	86.799	-6089.	-3992.	0.174
1250.	-2599718.	-1968803.	82.272	-5979.	-3906.	0.163
(2 sigma)	---	---	---	562.	516.	0.022
1300.	-2598503.	-1943590.	78.094	-5785.	-3827.	0.154
1350.	-2597165.	-1918426.	74.228	-5494.	-3757.	0.145
1400.	-2595688.	-1893314.	70.640	-5089.	-3699.	0.138
1450.	-2594057.	-1868258.	67.302	-4556.	-3659.	0.132
1500.	-2592254.	-1843260.	64.188	-3880.	-3639.	0.127
(2 sigma)	---	---	---	711.	556.	0.019
1550.	-2590263.	-1818326.	61.277	-3043.	-3644.	0.123
1600.	-2588065.	-1793459.	58.550	-2030.	-3679.	0.120
1650.	-2585642.	-1768665.	55.991	-824.	-3749.	0.119
1700.	-2633484.	-1743497.	53.571	594.	-3858.	0.119
1750.	-2630411.	-1717365.	51.261	2239.	-4013.	0.120
(2 sigma)	---	---	---	1601.	621.	0.019
1800.	-2627049.	-1691325.	49.081	4131.	-4218.	0.122
(2 sigma)	---	---	---	1907.	645.	0.019

Table 26. Thermophysical values for andalusite, Al_2SiO_5, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	83.694	50.069	-10312.	-101.630	51.4657
250.	106.213	71.256	-5544.	-93.432	51.5103
(2 sigma)	0.149	0.346	6.	0.345	0.0226
273.15	114.981	81.052	-2982.	-91.968	51.5332
298.15	123.374	91.492	0.	-91.492	51.5593
(2 sigma)	0.129	0.345	0.	0.345	0.0155
300.	123.954	92.257	229.	-91.494	51.5613
350.	137.744	112.444	6786.	-93.057	51.6179
400.	148.501	131.569	13953.	-96.687	51.6791
450.	156.958	149.568	21598.	-101.573	51.7443
500.	163.667	166.465	29620.	-107.226	51.8128
(2 sigma)	0.294	0.353	35.	0.345	0.0222
550.	169.038	182.326	37942.	-113.340	51.8841
600.	173.382	197.227	46506.	-119.716	51.9578
650.	176.937	211.250	55267.	-126.223	52.0335
700.	179.886	224.473	64190.	-132.773	52.1109
750.	182.375	236.971	73248.	-139.307	52.1898
(2 sigma)	0.313	0.377	88.	0.348	0.0230
800.	184.520	248.811	82422.	-145.784	52.2699
850.	186.413	260.056	91696.	-152.178	52.3511
900.	188.131	270.760	101060.	-158.471	52.4331
950.	189.737	280.975	110507.	-164.652	52.5158
1000.	191.283	290.747	120033.	-170.714	52.5992
(2 sigma)	0.517	0.387	133.	0.351	0.0189
1050.	192.814	300.117	129635.	-176.655	52.6831
1100.	194.366	309.122	139314.	-182.473	52.7675
1150.	195.972	317.797	149073.	-188.169	52.8523
1200.	197.659	326.173	158913.	-193.746	52.9374
1250.	199.450	334.278	168840.	-199.206	53.0227
(2 sigma)	0.603	0.399	195.	0.354	0.0312
1300.	201.366	342.137	178860.	-204.553	53.1083
1350.	203.425	349.775	188979.	-209.790	53.1941
1400.	205.643	357.213	199205.	-214.923	53.2800
1450.	208.034	364.470	209546.	-219.955	53.3661
1500.	210.609	371.566	220012.	-224.891	53.4523
(2 sigma)	1.993	0.420	300.	0.357	0.0538
1550.	213.381	378.516	230611.	-229.735	53.5386
1600.	216.358	385.337	241353.	-234.491	53.6250
1650.	219.549	392.043	252250.	-239.164	53.7115
1700.	222.962	398.647	263312.	-243.758	53.7980
1750.	226.605	405.163	274550.	-248.277	53.8846
(2 sigma)	4.807	0.723	1013.	0.361	0.0796
1800.	230.484	411.600	285976.	-252.724	53.9712
(2 sigma)	5.534	0.845	1259.	0.364	0.0849

Table 27. Thermochemical properties of andalusite, Al_2SiO_5, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-2589464.	-2492795.	651.051	-6176.	-6016.	1.571
250.	-2591434.	-2468382.	515.740	-6190.	-5976.	1.249
(2 sigma)	---	---	---	500.	462.	0.097
273.15	-2592084.	-2456957.	469.845	-6205.	-5955.	1.139
298.15	-2592626.	-2444564.	428.277	-6217.	-5932.	1.039
(2 sigma)	---	---	---	500.	456.	0.080
300.	-2592660.	-2443645.	425.476	-6218.	-5930.	1.032
350.	-2593307.	-2418752.	360.979	-6229.	-5881.	0.878
400.	-2593519.	-2393796.	312.598	-6234.	-5831.	0.761
450.	-2593410.	-2368835.	274.967	-6252.	-5779.	0.671
500.	-2593070.	-2343898.	244.865	-6303.	-5724.	0.598
(2 sigma)	---	---	---	504.	438.	0.046
550.	-2592568.	-2319004.	220.241	-6401.	-5662.	0.538
600.	-2591961.	-2294161.	199.724	-6558.	-5589.	0.487
650.	-2591291.	-2269371.	182.369	-6781.	-5499.	0.442
700.	-2590596.	-2244634.	167.497	-7077.	-5390.	0.402
750.	-2589901.	-2219947.	154.611	-7447.	-5257.	0.366
(2 sigma)	---	---	---	512.	429.	0.030
800.	-2589230.	-2195306.	143.339	-7892.	-5097.	0.333
850.	-2588602.	-2170705.	133.395	-9121.	-4902.	0.301
900.	-2588029.	-2146140.	124.559	-9286.	-4649.	0.270
950.	-2608781.	-2120957.	116.618	-9450.	-4387.	0.241
1000.	-2608080.	-2095300.	109.447	-9611.	-4116.	0.215
(2 sigma)	---	---	---	518.	440.	0.023
1050.	-2607341.	-2069679.	102.961	-9766.	-3837.	0.191
1100.	-2606564.	-2044094.	97.066	-9909.	-3552.	0.169
1150.	-2605743.	-2018546.	91.685	-10034.	-3260.	0.148
1200.	-2604872.	-1993034.	86.754	-10136.	-2963.	0.129
1250.	-2603945.	-1967559.	82.220	-10206.	-2663.	0.111
(2 sigma)	---	---	---	533.	470.	0.020
1300.	-2602954.	-1942123.	78.035	-10237.	-2360.	0.095
1350.	-2601890.	-1916727.	74.163	-10219.	-2057.	0.080
1400.	-2600744.	-1891371.	70.568	-10145.	-1756.	0.066
1450.	-2599505.	-1866058.	67.223	-10004.	-1459.	0.053
1500.	-2598162.	-1840789.	64.102	-9788.	-1168.	0.041
(2 sigma)	---	---	---	583.	517.	0.018
1550.	-2596705.	-1815567.	61.184	-9485.	-885.	0.030
1600.	-2595121.	-1790394.	58.450	-9086.	-614.	0.020
1650.	-2593399.	-1765272.	55.884	-8581.	-357.	0.011
1700.	-2642035.	-1739755.	53.456	-7957.	-116.	0.004
1750.	-2639855.	-1713249.	51.138	-7205.	104.	-0.003
(2 sigma)	---	---	---	1139.	578.	0.017
1800.	-2637493.	-1686808.	48.950	-6313.	300.	-0.009
(2 sigma)	---	---	---	1367.	595.	0.017

Table 28. Thermophysical values for kyanite, Al_2SiO_5, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	80.961	41.807	-10116.	-92.388	44.1175
250.	104.208	62.455	-5468.	-84.326	44.1618
(2 sigma)	0.145	0.303	6.	0.303	0.0306
273.15	113.385	72.091	-2947.	-82.881	44.1833
298.15	122.219	82.410	0.	-82.410	44.2071
(2 sigma)	0.121	0.302	0.	0.302	0.0229
300.	122.831	83.168	227.	-82.413	44.2089
350.	137.448	103.246	6748.	-83.965	44.2584
400.	148.930	122.380	13919.	-87.581	44.3098
450.	158.009	140.466	21602.	-92.462	44.3630
500.	165.247	157.503	29690.	-98.123	44.4175
(2 sigma)	0.307	0.311	38.	0.302	0.0173
550.	171.070	173.535	38103.	-104.257	44.4733
600.	175.801	188.630	46779.	-110.666	44.5301
650.	179.689	202.860	55669.	-117.216	44.5878
700.	182.926	216.299	64737.	-123.818	44.6461
750.	185.667	229.015	73953.	-130.411	44.7052
(2 sigma)	0.351	0.332	89.	0.304	0.0158
800.	188.032	241.075	83297.	-136.954	44.7647
850.	190.121	252.538	92752.	-143.418	44.8247
900.	192.015	263.460	102306.	-149.786	44.8850
950.	193.780	273.889	111951.	-156.046	44.9457
1000.	195.471	283.872	121683.	-162.189	45.0067
(2 sigma)	0.534	0.339	140.	0.305	0.0144
1050.	197.137	293.449	131498.	-168.213	45.0679
1100.	198.816	302.659	141397.	-174.116	45.1292
1150.	200.543	311.534	151380.	-179.899	45.1908
1200.	202.346	320.107	161452.	-185.564	45.2524
1250.	204.251	328.406	171617.	-191.112	45.3142
(2 sigma)	0.875	0.350	194.	0.306	0.0288
1300.	206.280	336.455	181879.	-196.548	45.3761
1350.	208.451	344.281	192247.	-201.876	45.4381
1400.	210.782	351.903	202727.	-207.098	45.5001
1450.	213.287	359.343	213328.	-212.220	45.5622
1500.	215.979	366.619	224059.	-217.246	45.6244
(2 sigma)	2.969	0.452	453.	0.309	0.0500
1550.	218.871	373.747	234929.	-222.180	45.6866
1600.	221.972	380.744	245949.	-227.026	45.7488
1650.	225.293	387.625	257130.	-231.789	45.8111
1700.	228.840	394.403	268483.	-236.472	45.8734
1750.	232.623	401.090	280018.	-241.080	45.9357
(2 sigma)	6.734	1.039	1557.	0.326	0.0731
1800.	236.647	407.699	291749.	-245.617	45.9980
(2 sigma)	7.687	1.228	1908.	0.335	0.0778

Table 29. Thermochemical properties of kyanite, Al_2SiO_5, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-2592988.	-2494666.	651.539	-9699.	-7887.	2.060
250.	-2595078.	-2469826.	516.041	-9834.	-7419.	1.550
(2 sigma)	---	---	---	520.	491.	0.103
273.15	-2595769.	-2458195.	470.082	-9891.	-7193.	1.375
298.15	-2596346.	-2445577.	428.455	-9937.	-6944.	1.217
(2 sigma)	---	---	---	520.	487.	0.085
300.	-2596382.	-2444641.	425.650	-9940.	-6925.	1.206
350.	-2597064.	-2419289.	361.059	-9986.	-6418.	0.958
400.	-2597272.	-2393874.	312.608	-9987.	-5908.	0.772
450.	-2597126.	-2368455.	274.923	-9968.	-5399.	0.627
500.	-2596719.	-2343067.	244.778	-9953.	-4893.	0.511
(2 sigma)	---	---	---	524.	472.	0.049
550.	-2596127.	-2317729.	220.119	-9960.	-4387.	0.417
600.	-2595408.	-2292451.	199.575	-10005.	-3878.	0.338
650.	-2594609.	-2267236.	182.197	-10099.	-3364.	0.270
700.	-2593769.	-2242085.	167.306	-10250.	-2841.	0.212
750.	-2592916.	-2216995.	154.405	-10462.	-2305.	0.161
(2 sigma)	---	---	---	531.	463.	0.032
800.	-2592075.	-2191961.	143.120	-10736.	-1752.	0.114
850.	-2591265.	-2166979.	133.166	-11785.	-1176.	0.072
900.	-2590503.	-2142043.	124.321	-11759.	-552.	0.032
950.	-2611057.	-2116501.	116.373	-11725.	70.	-0.004
1000.	-2610149.	-2090495.	109.196	-11681.	689.	-0.036
(2 sigma)	---	---	---	534.	469.	0.025
1050.	-2609198.	-2064535.	102.705	-11623.	1306.	-0.065
1100.	-2608201.	-2038622.	96.806	-11547.	1920.	-0.091
1150.	-2607155.	-2012755.	91.422	-11447.	2530.	-0.115
1200.	-2606053.	-1986935.	86.489	-11317.	3135.	-0.136
1250.	-2604889.	-1961162.	81.952	-11149.	3734.	-0.156
(2 sigma)	---	---	---	546.	490.	0.020
1300.	-2603655.	-1935437.	77.767	-10937.	4326.	-0.174
1350.	-2602342.	-1909761.	73.893	-10671.	4908.	-0.190
1400.	-2600942.	-1884136.	70.298	-10343.	5479.	-0.204
1450.	-2599443.	-1858562.	66.953	-9943.	6037.	-0.217
1500.	-2597835.	-1833041.	63.832	-9461.	6580.	-0.229
(2 sigma)	---	---	---	696.	522.	0.018
1550.	-2596106.	-1807576.	60.915	-8887.	7106.	-0.239
1600.	-2594245.	-1782169.	58.182	-8210.	7611.	-0.248
1650.	-2592239.	-1756822.	55.616	-7420.	8094.	-0.256
1700.	-2640584.	-1731089.	53.190	-6506.	8550.	-0.263
1750.	-2638107.	-1704374.	50.873	-5457.	8978.	-0.268
(2 sigma)	---	---	---	1665.	585.	0.017
1800.	-2635440.	-1677734.	48.687	-4260.	9374.	-0.272
(2 sigma)	---	---	---	2003.	610.	0.018

Table 30. Thermophysical values for sillimanite, Al_2SiO_5, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	86.686	53.855	-10377.	-105.738	49.9871
250.	106.536	75.362	-5539.	-97.518	50.0005
(2 sigma)	0.133	0.334	6.	0.333	0.0219
273.15	114.855	85.165	-2975.	-96.057	50.0085
298.15	123.013	95.581	0.	-95.581	50.0183
(2 sigma)	0.116	0.333	0.	0.333	0.0165
300.	123.583	96.344	228.	-95.584	50.0190
350.	137.289	116.464	6763.	-97.141	50.0419
400.	148.127	135.533	13909.	-100.760	50.0684
450.	156.678	153.493	21538.	-105.632	50.0980
500.	163.450	170.365	29547.	-111.270	50.1303
(2 sigma)	0.230	0.338	28.	0.333	0.0144
550.	168.852	186.206	37860.	-117.370	50.1648
600.	173.204	201.091	46415.	-123.733	50.2012
650.	176.760	215.100	55167.	-130.228	50.2391
700.	179.721	228.311	64081.	-136.766	50.2785
750.	182.248	240.799	73132.	-143.289	50.3190
(2 sigma)	0.345	0.351	74.	0.334	0.0143
800.	184.470	252.633	82301.	-149.757	50.3604
850.	186.492	263.878	91576.	-156.142	50.4027
900.	188.403	274.592	100948.	-162.427	50.4456
950.	190.273	284.828	110415.	-168.602	50.4892
1000.	192.164	294.636	119976.	-174.660	50.5332
(2 sigma)	0.452	0.368	139.	0.335	0.0109
1050.	194.126	304.059	129633.	-180.599	50.5777
1100.	196.204	313.137	139390.	-186.418	50.6225
1150.	198.433	321.907	149256.	-192.120	50.6676
1200.	200.847	330.403	159237.	-197.705	50.7130
1250.	203.472	338.654	169344.	-203.179	50.7586
(2 sigma)	0.892	0.380	188.	0.337	0.0170
1300.	206.334	346.689	179588.	-208.545	50.8044
1350.	209.453	354.534	189982.	-213.807	50.8503
1400.	212.848	362.212	200538.	-218.971	50.8964
1450.	216.535	369.745	211271.	-224.040	50.9425
1500.	220.529	377.152	222197.	-229.021	50.9888
(2 sigma)	2.830	0.474	458.	0.340	0.0303
1550.	224.842	384.452	233329.	-233.917	51.0351
1600.	229.488	391.663	244686.	-238.734	51.0816
1650.	234.475	398.800	256284.	-243.477	51.1280
1700.	239.813	405.879	268140.	-248.149	51.1746
1750.	245.511	412.912	280271.	-252.757	51.2211
(2 sigma)	6.160	1.001	1488.	0.353	0.0456
1800.	251.576	419.912	292697.	-257.303	51.2677
(2 sigma)	6.994	1.171	1809.	0.360	0.0488

Table 31. Thermochemical properties of sillimanite, Al_2SiO_5, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

T K	Formation from the Elements			Formation from the Oxides		
	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-2585805.	-2489893.	650.293	-2517.	-3114.	0.813
250.	-2587706.	-2465680.	515.175	-2462.	-3274.	0.684
(2 sigma)	---	---	---	537.	505.	0.106
273.15	-2588354.	-2454351.	469.347	-2475.	-3349.	0.640
298.15	-2588902.	-2442060.	427.839	-2494.	-3428.	0.601
(2 sigma)	---	---	---	537.	500.	0.088
300.	-2588937.	-2441149.	425.042	-2496.	-3433.	0.598
350.	-2589606.	-2416458.	360.636	-2528.	-3587.	0.535
400.	-2589839.	-2391702.	312.324	-2554.	-3737.	0.488
450.	-2589747.	-2366938.	274.747	-2589.	-3882.	0.451
500.	-2589418.	-2342197.	244.687	-2652.	-4023.	0.420
(2 sigma)	---	---	---	539.	485.	0.051
550.	-2588927.	-2317498.	220.097	-2760.	-4155.	0.395
600.	-2588328.	-2292848.	199.610	-2925.	-4276.	0.372
650.	-2587668.	-2268251.	182.279	-3158.	-4379.	0.352
700.	-2586981.	-2243706.	167.427	-3462.	-4462.	0.333
750.	-2586294.	-2219211.	154.559	-3840.	-4521.	0.315
(2 sigma)	---	---	---	543.	479.	0.033
800.	-2585628.	-2194760.	143.303	-4289.	-4552.	0.297
850.	-2584999.	-2170351.	133.373	-5518.	-4548.	0.279
900.	-2584417.	-2145977.	124.549	-5674.	-4486.	0.260
950.	-2605150.	-2120986.	116.620	-5818.	-4416.	0.243
1000.	-2604413.	-2095523.	109.459	-5945.	-4339.	0.227
(2 sigma)	---	---	---	550.	489.	0.026
1050.	-2603620.	-2070097.	102.982	-6045.	-4256.	0.212
1100.	-2602765.	-2044711.	97.095	-6110.	-4169.	0.198
1150.	-2601836.	-2019366.	91.722	-6128.	-4080.	0.185
1200.	-2600825.	-1994062.	86.799	-6089.	-3992.	0.174
1250.	-2599718.	-1968803.	82.272	-5979.	-3906.	0.163
(2 sigma)	---	---	---	562.	516.	0.022
1300.	-2598503.	-1943590.	78.094	-5785.	-3827.	0.154
1350.	-2597165.	-1918426.	74.228	-5494.	-3757.	0.145
1400.	-2595688.	-1893314.	70.640	-5089.	-3699.	0.138
1450.	-2594057.	-1868258.	67.302	-4556.	-3659.	0.132
1500.	-2592254.	-1843260.	64.188	-3880.	-3639.	0.127
(2 sigma)	---	---	---	711.	556.	0.019
1550.	-2590263.	-1818326.	61.277	-3043.	-3644.	0.123
1600.	-2588065.	-1793459.	58.550	-2030.	-3679.	0.120
1650.	-2585642.	-1768665.	55.991	-824.	-3749.	0.119
1700.	-2633484.	-1743497.	53.571	594.	-3858.	0.119
1750.	-2630411.	-1717365.	51.261	2239.	-4013.	0.120
(2 sigma)	---	---	---	1601.	621.	0.019
1800.	-2627049.	-1691325.	49.081	4131.	-4218.	0.122
(2 sigma)	---	---	---	1907.	645.	0.019

Table 32. Thermophysical values for kaolinite, $Al_2Si_2O_5(OH)_4$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T	C_p°	S°	$H_T^\circ - H_{298}^\circ$	$[G_T^\circ - H_{298}^\circ]/T$	V°
K	J/(mol K)	J/(mol K)	J/mol	J/(mol K)	cm^3/mol
200.	173.618	120.875	-20951.	-225.629	99.1354
250.	215.926	164.429	-11152.	-209.038	99.3145
(2 sigma)	0.314	0.478	17.	0.472	0.3428
273.150	231.375	184.241	-5971.	-206.100	99.3974
298.150	245.941	205.147	0.	-205.147	99.4870
(2 sigma)	0.406	0.473	0.	0.473	0.3368
300.	246.944	206.672	456.	-205.152	99.4936
350.	270.854	246.607	13425.	-208.251	99.6727
400.	289.949	284.066	27462.	-215.412	99.8518
450.	305.604	319.150	42363.	-225.011	100.0310
500.	318.700	352.046	57979.	-236.087	100.2101
(2 sigma)	1.171	0.577	147.	0.473	0.4253
550.	329.832	382.957	74200.	-248.048	100.3892
600.	339.419	412.077	90937.	-260.515	100.5683
650.	347.762	439.582	108121.	-273.242	100.7474
700.	355.088	465.628	125696.	-286.062	100.9265
750.	361.570	490.352	143616.	-298.864	101.1056
(2 sigma)	1.655	0.994	492.	0.522	0.6738
800.	367.340	513.875	161841.	-311.573	101.2848
850.	372.506	536.302	180340.	-324.138	101.4639
900.	377.153	557.728	199083.	-336.524	101.6430
950.	381.349	578.234	218048.	-348.710	101.8221
1000.	385.152	597.893	237212.	-360.681	102.0012
(2 sigma)	2.223	1.393	893.	0.643	0.9680
1050.	388.609	616.769	256557.	-372.429	102.1803
1100.	391.759	634.921	276067.	-383.951	102.3594
1150.	394.637	652.400	295728.	-395.245	302.5386
1200.	397.271	669.252	315527.	-406.313	302.7177
1250.	399.686	685.519	335452.	-417.158	102.8968
(2 sigma)	3.520	1.774	1422.	0.793	1.2767

Table 33. Thermochemical properties of kaolinite, $Al_2Si_2O_5(OH)_4$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-4124584.	-3909930.	1021.168	---	---	---
250.	-4129707.	-3855648.	805.593	---	---	---
(2 sigma)	---	---	---	---	---	---
273.150	-4131697.	-3830179.	732.447	-51821.	-34874.	6.669
298.150	-4133615.	-3802496.	666.181	-53707.	-33239.	5.823
(2 sigma)	---	---	---	168.	195.	0.034
300.	-4133749.	-3800441.	661.715	-53842.	-33111.	5.765
350.	-4136942.	-3744627.	558.855	-57323.	-29377.	4.384
400.	-4139465.	-3688403.	481.656	-140073.	-19358.	2.528
450.	-4141459.	-3631895.	421.579	-139022.	-4330.	0.503
500.	-4143029.	-3575189.	373.497	-137867.	10574.	-1.105
(2 sigma)	---	---	---	227.	259.	0.027
550.	-4144264.	-3518343.	334.144	-136649.	25360.	-2.408
600.	-4145234.	-3461397.	301.341	-135401.	40033.	-3.485
650.	-4145996.	-3404378.	273.579	-134149.	54602.	-4.388
700.	-4146600.	-3347307.	249.779	-132913.	69074.	-5.154
750.	-4147088.	-3290197.	229.150	-131713.	83460.	-5.813
(2 sigma)	---	---	---	524.	393.	0.027
800.	-4147495.	-3233057.	211.097	-130561.	97767.	-6.384
850.	-4147854.	-3175894.	195.167	-130896.	112014.	-6.884
900.	-4148193.	-3118710.	181.005	-129033.	126250.	-7.327
950.	-4127077.	-3105812.	170.769	-127121.	140380.	-7.719
1000.	-4124533.	-3052127.	159.427	-125173.	154409.	-8.065
(2 sigma)	---	---	---	912.	636.	0.033
1050.	-4121899.	-2998571.	149.171	-123201.	168339.	-8.374
1100.	-4119188.	-2945142.	139.853	-121217.	182176.	-8.651
1150.	-4116411.	-2891838.	131.351	-119230.	195922.	-8.899
1200.	-4113576.	-2838657.	123.563	-117249.	209582.	-9.123
1250.	-4110691.	-2785594.	116.404	-115280.	223159.	-9.325
(2 sigma)	---	---	---	1434.	981.	0.041

Table 34. Thermophysical values for dickite, $Al_2Si_2O_5(OH)_4$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	168.792	115.478	-20284.	-216.900	98.9368
250.	208.625	157.588	-10812.	-200.835	99.1218
(2 sigma)	0.584	3.231	32.	3.229	0.2185
273.15	224.230	176.756	-5798.	-197.984	99.2075
298.15	239.361	197.058	0.	-197.058	99.3000
(2 sigma)	0.764	3.229	0.	3.229	0.1801
300.	240.416	198.542	444.	-197.063	99.3068
350.	265.995	237.593	13126.	-200.088	99.4918
400.	286.869	274.519	26965.	-207.107	99.6768
450.	304.136	309.336	41753.	-216.550	99.8618
500.	318.591	342.150	57332.	-227.486	100.0468
(2 sigma)	2.151	3.297	276.	3.231	0.5495
550.	330.811	373.104	73575.	-239.330	100.2318
600.	341.226	402.346	90383.	-251.708	100.4168
650.	350.159	430.021	107673.	-264.369	100.6018
700.	357.862	456.259	125379.	-277.147	100.7868
750.	364.529	481.182	143442.	-289.925	100.9718
(2 sigma)	2.820	3.621	891.	3.262	1.1761
800.	370.315	504.897	161817.	-302.626	101.1568
850.	375.344	527.502	180461.	-315.194	101.3418
900.	379.720	549.083	199340.	-327.593	101.5268
950.	383.524	569.717	218424.	-339.798	101.7118
1000.	386.827	589.475	237684.	-351.791	101.8968
(2 sigma)	3.397	3.984	1529.	3.336	1.8143
1050.	389.686	608.420	257099.	-363.564	102.0818
1100.	392.152	626.606	276646.	-375.109	102.2668
1150.	394.265	644.086	296308.	-386.427	102.4518
1200.	396.063	660.905	316068.	-397.515	102.6368
1250.	397.575	677.104	335910.	-408.377	102.8218
(2 sigma)	5.430	4.305	2252.	3.434	2.4550

Table 35. Thermochemical properties of dickite, $Al_2Si_2O_5(OH)_4$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-4122604.	-3906870.	1020.369	---	---	---
250.	-4128053.	-3852284.	804.890	---	---	---
(2 sigma)	---	---	---	---	---	---
273.15	-4130211.	-3826649.	731.772	-50335.	-31344.	5.994
298.15	-4132302.	-3798770.	665.528	-52393.	-29513.	5.171
(2 sigma)	---	---	---	1239.	1569.	0.275
300.	-4132447.	-3796700.	661.064	-52540.	-29371.	5.114
350.	-4135926.	-3740456.	558.232	-56308.	-25206.	3.762
400.	-4138648.	-3683767.	481.050	-139256.	-14722.	1.922
450.	-4140754.	-3626774.	420.985	-138317.	791.	-0.092
500.	-4142363.	-3569575.	372.911	-137200.	16189.	-1.691
(2 sigma)	---	---	---	1270.	2036.	0.213
550.	-4143575.	-3512234.	333.564	-135960.	31468.	-2.989
600.	-4144474.	-3454798.	300.767	-134641.	46631.	-4.060
650.	-4145130.	-3397297.	273.010	-133283.	61682.	-4.957
700.	-4145604.	-3339753.	249.215	-131917.	76629.	-5.718
750.	-4145947.	-3282179.	228.591	-130572.	91478.	-6.371
(2 sigma)	---	---	---	1526.	2742.	0.191
800.	-4146206.	-3224586.	210.544	-129272.	106238.	-6.937
850.	-4146419.	-3166978.	194.619	-129461.	120930.	-7.431
900.	-4146622.	-3109358.	180.462	-127462.	135601.	-7.870
950.	-4125387.	-3096031.	170.232	-125431.	150161.	-8.256
1000.	-4122746.	-3041923.	158.894	-123386.	164612.	-8.598
(2 sigma)	---	---	---	1968.	3559.	0.186
1050.	-4120044.	-2987948.	148.642	-121345.	178962.	-8.903
1100.	-4117296.	-2934103.	139.329	-119324.	193215.	-9.175
1150.	-4114517.	-2880384.	130.831	-117336.	207377.	-9.419
1200.	-4111721.	-2826785.	123.047	-115394.	221453.	-9.640
1250.	-4108919.	-2773304.	115.890	-113509.	235449.	-9.839
(2 sigma)	---	---	---	2571.	4467.	0.187

Table 36. Thermophysical values for halloysite, $Al_2Si_2O_5(OH)_4$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	173.879	119.323	-20883.	-223.736	99.0368
250.	215.076	162.787	-11105.	-207.209	99.2218
(2 sigma)	0.609	3.231	33.	3.229	1.2921
273.15	230.388	182.517	-5945.	-204.283	99.3075
298.15	244.925	203.334	0.	-203.334	99.4000
(2 sigma)	0.787	3.229	0.	3.229	1.2861
300.	245.929	204.852	454.	-203.339	99.4068
350.	269.953	244.639	13374.	-206.426	99.5918
400.	289.211	281.988	27370.	-213.562	99.7768
450.	304.997	316.993	42238.	-223.130	99.9618
500.	318.165	349.829	57827.	-234.176	100.1468
(2 sigma)	2.342	3.308	297.	3.231	1.3869
550.	329.303	380.690	74021.	-246.107	100.3318
600.	338.828	409.762	90730.	-258.545	100.5168
650.	347.050	437.215	107882.	-271.243	100.7018
700.	354.200	463.202	125417.	-284.034	100.8868
750.	360.456	487.857	143287.	-296.808	101.0718
(2 sigma)	3.333	3.689	975.	3.267	1.7335
800.	365.957	511.300	161450.	-309.487	101.2568
850.	370.813	533.635	179872.	-322.020	101.4418
900.	375.115	554.954	198522.	-334.373	101.6268
950.	378.935	575.340	217375.	-346.523	101.8118
1000.	382.333	594.865	236409.	-358.456	101.9968
(2 sigma)	5.036	4.180	1799.	3.356	2.2166
1050.	385.360	613.593	255603.	-370.162	102.1818
1100.	388.057	631.584	274939.	-381.639	102.3668
1150.	390.461	648.888	294403.	-392.885	102.5518
1200.	392.602	665.552	313981.	-403.901	102.7368
1250.	394.507	681.618	333660.	-414.690	102.9218
(2 sigma)	8.439	4.825	3071.	3.484	2.7656

Table 37. Thermochemical properties of halloysite, $Al_2Si_2O_5(OH)_4$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-4105755.	-3890790.	1016.169	---	---	---
250.	-4110899.	-3836430.	801.578	---	---	---
(2 sigma)	---	---	---	---	---	---
273.15	-4112911.	-3810922.	728.764	-33035.	-15617.	2.986
298.15	-4114854.	-3783194.	662.799	-34946.	-13937.	2.442
(2 sigma)	---	---	---	1198.	1537.	0.269
300.	-4114989.	-3781136.	658.354	-35083.	-13806.	2.404
350.	-4118231.	-3725227.	555.959	-38613.	-9977.	1.489
400.	-4120796.	-3668901.	479.109	-121403.	143.	-0.019
450.	-4122822.	-3612288.	419.303	-120385.	15277.	-1.773
500.	-4124421.	-3555473.	371.437	-119259.	30291.	-3.164
(2 sigma)	---	---	---	1234.	2011.	0.210
550.	-4125682.	-3498514.	332.261	-118067.	45189.	-4.292
600.	-4126680.	-3441453.	299.605	-116847.	59976.	-5.221
650.	-4127474.	-3384318.	271.967	-115627.	74662.	-6.000
700.	-4128118.	-3327127.	248.273	-114431.	89254.	-6.660
750.	-4128655.	-3269894.	227.735	-113280.	103763.	-7.227
(2 sigma)	---	---	---	1545.	2728.	0.190
800.	-4129125.	-3212627.	209.763	-112191.	118197.	-7.717
850.	-4129561.	-3155333.	193.903	-112603.	132575.	-8.147
900.	-4129993.	-3098013.	179.804	-110833.	146946.	-8.529
950.	-4108988.	-3084974.	169.624	-109032.	161218.	-8.864
1000.	-4106575.	-3031140.	158.330	-107214.	175395.	-9.162
(2 sigma)	---	---	---	2162.	3563.	0.186
1050.	-4104093.	-2977429.	148.119	-105395.	189481.	-9.426
1100.	-4101556.	-2923838.	138.841	-103584.	203480.	-9.662
1150.	-4098975.	-2870363.	130.376	-101794.	217397.	-9.874
1200.	-4096361.	-2817001.	122.621	-100034.	231237.	-10.065
1250.	-4093722.	-2763749.	115.491	-98312.	245005.	-10.238
(2 sigma)	---	---	---	3296.	4517.	0.189

Table 38. Thermophysical values for pyrophyllite, $Al_2Si_4O_{10}(OH)_2$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	208.741	138.995	-24944.	-263.715	127.5844
250.	256.332	190.835	-13284.	-243.970	127.6066
(2 sigma)	0.355	1.023	15.	1.022	0.2819
273.15	275.484	214.385	-7124.	-240.467	127.6204
298.15	294.131	239.330	0.	-239.330	127.6374
(2 sigma)	0.304	1.022	0.	1.022	0.1460
300.	295.431	241.154	545.	-239.336	127.6387
350.	326.835	289.142	16131.	-243.054	127.6792
400.	352.103	334.494	33127.	-251.677	127.7268
450.	372.607	377.190	51262.	-263.275	127.7803
500.	389.424	417.347	70326.	-276.695	127.8389
(2 sigma)	1.036	1.053	109.	1.023	0.1633
550.	403.375	455.138	90157.	-291.216	127.9018
600.	415.089	490.752	110626.	-306.375	127.9683
650.	425.051	524.381	131636.	-321.863	128.0379
700.	433.642	556.202	153109.	-337.476	128.1101
750.	441.160	586.382	174983.	-353.072	128.1845
(2 sigma)	3.253	1.383	569.	1.040	0.5781
800.	447.846	615.072	197211.	-368.558	128.2608
850.	453.895	642.406	219757.	-383.869	128.3386
900.	459.466	668.510	242592.	-398.963	128.4178
950.	464.692	693.493	265698.	-413.812	128.4981
1000.	469.681	717.456	289058.	-428.399	128.5794
(2 sigma)	4.928	2.252	1549.	1.132	1.5153
1050.	474.528	740.490	312663.	-442.715	128.6614
1100.	479.310	762.675	336509.	-456.758	128.7442
1150.	484.095	784.087	360594.	-470.527	128.8275
1200.	488.940	804.792	384920.	-484.026	128.9114
1250.	493.895	824.852	409490.	-497.259	128.9956
(2 sigma)	6.925	3.199	2763.	1.346	2.6320

Table 39. Thermochemical properties of pyrophyllite, $Al_2Si_4O_{10}(OH)_2$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

T	Formation from the Elements			Formation from the Oxides		
K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-5635721.	-5390571.	1407.872	---	---	---
250.	-5639805.	-5328777.	1113.386	---	---	---
(2 sigma)	---	---	---	---	---	---
273.15	-5641174.	-5299912.	1013.505	-37075.	-25059.	4.792
298.15	-5642319.	-5268625.	923.041	-38094.	-23913.	4.189
(2 sigma)	---	---	---	983.	807.	0.141
300.	-5642391.	-5266306.	916.945	-38166.	-23825.	4.148
350.	-5643738.	-5203504.	776.580	-39990.	-21287.	3.177
400.	-5644099.	-5140578.	671.290	-81384.	-15600.	2.037
450.	-5643689.	-5077655.	589.398	-80859.	-7408.	0.860
500.	-5642678.	-5014812.	523.893	-80309.	723.	-0.076
(2 sigma)	---	---	---	998.	735.	0.077
550.	-5641202.	-4952094.	470.310	-79792.	8801.	-0.836
600.	-5639370.	-4889526.	425.671	-79355.	16835.	-1.466
650.	-5637267.	-4827122.	387.912	-79035.	24837.	-1.996
700.	-5634960.	-4764889.	355.560	-78857.	32819.	-2.449
750.	-5632502.	-4702826.	327.534	-78841.	40795.	-2.841
(2 sigma)	---	---	---	1167.	724.	0.050
800.	-5629937.	-4640931.	303.021	-78999.	48775.	-3.185
850.	-5627297.	-4579199.	281.403	-82188.	56791.	-3.490
900.	-5624608.	-4517623.	262.196	-81019.	64933.	-3.769
950.	-5643146.	-4455551.	244.983	-79770.	73007.	-4.014
1000.	-5640138.	-4393123.	229.473	-78449.	81014.	-4.232
(2 sigma)	---	---	---	1869.	903.	0.047
1050.	-5637004.	-4330849.	215.448	-77059.	88954.	-4.425
1100.	-5633743.	-4268727.	202.705	-75601.	96825.	-4.598
1150.	-5630350.	-4206756.	191.077	-74071.	104629.	-4.752
1200.	-5626817.	-4144936.	180.424	-72463.	112364.	-4.891
1250.	-5623134.	-4083266.	170.630	-70771.	120031.	-5.016
(2 sigma)	---	---	---	2960.	1403.	0.059

Table 40. Thermophysical values for the elemental phase graphite (C) at 1.01325 bars (1 atm). The sources of data are given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	6.646	2.872	-710.	-6.420	---
250.	7.087	4.366	-374.	-5.863	---
(2 sigma)	---	---	---	---	---
273.15	7.728	5.021	-203.	-5.764	---
298.15	8.532	5.732	0.	-5.732	---
(2 sigma)	---	---	---	---	---
300.	8.594	5.785	16.	-5.732	---
350.	10.296	7.237	488.	-5.843	---
400.	11.923	8.720	1044.	-6.109	---
450.	13.397	10.211	1678.	-6.482	---
500.	14.704	11.691	2381.	-6.929	---
(2 sigma)	---	---	---	---	---
550.	15.855	13.148	3146.	-7.429	---
600.	16.865	14.572	3964.	-7.965	---
650.	17.750	15.957	4830.	-8.527	---
700.	18.528	17.302	5737.	-9.106	---
750.	19.212	18.604	6681.	-9.696	---
(2 sigma)	---	---	---	---	---
800.	19.814	19.863	7657.	-10.292	---
850.	20.346	21.081	8661.	-10.891	---
900.	20.817	22.257	9691.	-11.490	---
950.	21.234	23.394	10742.	-12.087	---
1000.	21.604	24.493	11813.	-12.680	---
(2 sigma)	---	---	---	---	---
1050.	21.933	25.555	12902.	-13.268	---
1100.	22.226	26.583	14006.	-13.850	---
1150.	22.488	27.576	15124.	-14.425	---
1200.	22.721	28.538	16254.	-14.993	---
1250.	22.931	29.470	17396.	-15.554	---
(2 sigma)	---	---	---	---	---
1300.	23.119	30.373	18547.	-16.106	---
1350.	23.288	31.249	19707.	-16.651	---
1400.	23.441	32.099	20876.	-17.188	---
1450.	23.579	32.924	22051.	-17.716	---
1500.	23.704	33.725	23233.	-18.237	---
(2 sigma)	---	---	---	---	---
1550.	23.819	34.505	24421.	-18.749	---
1600.	23.924	35.262	25615.	-19.253	---
1650.	24.021	36.000	26814.	-19.749	---
1700.	24.111	36.719	28017.	-20.238	---
1750.	24.195	37.419	29225.	-20.719	---
(2 sigma)	---	---	---	---	---
1800.	24.275	38.101	30436.	-21.192	---
(2 sigma)	---	---	---	---	---

Table 41. Thermochemical properties of the elemental phase graphite (C) at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	$\log K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	$\log K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	0.	0.	0.	---	---	---
250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
273.15	0.	0.	0.	---	---	---
298.15	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
300.	0.	0.	0.	---	---	---
350.	0.	0.	0.	---	---	---
400.	0.	0.	0.	---	---	---
450.	0.	0.	0.	---	---	---
500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
550.	0.	0.	0.	---	---	---
600.	0.	0.	0.	---	---	---
650.	0.	0.	0.	---	---	---
700.	0.	0.	0.	---	---	---
750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
800.	0.	0.	0.	---	---	---
850.	0.	0.	0.	---	---	---
900.	0.	0.	0.	---	---	---
950.	0.	0.	0.	---	---	---
1000.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1050.	0.	0.	0.	---	---	---
1100.	0.	0.	0.	---	---	---
1150.	0.	0.	0.	---	---	---
1200.	0.	0.	0.	---	---	---
1250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1300.	0.	0.	0.	---	---	---
1350.	0.	0.	0.	---	---	---
1400.	0.	0.	0.	---	---	---
1450.	0.	0.	0.	---	---	---
1500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1550.	0.	0.	0.	---	---	---
1600.	0.	0.	0.	---	---	---
1650.	0.	0.	0.	---	---	---
1700.	0.	0.	0.	---	---	---
1750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1800.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---

Table 42. Thermophysical values for carbon monoxide (CO, ideal gas) at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	29.751	185.853	-2872.	-200.211	---
250.	29.181	192.417	-1401.	-198.022	---
(2 sigma)	---	---	---	---	---
273.15	29.093	194.997	-727.	-197.658	---
298.15	29.069	197.544	0.	-197.544	---
(2 sigma)	---	---	---	---	---
300.	29.070	197.723	54.	-197.544	---
350.	29.171	202.210	1509.	-197.898	---
400.	29.378	206.118	2973.	-198.687	---
450.	29.644	209.593	4448.	-199.709	---
500.	29.941	212.732	5937.	-200.857	---
(2 sigma)	---	---	---	---	---
550.	30.254	215.600	7442.	-202.069	---
600.	30.575	218.246	8963.	-203.308	---
650.	30.899	220.706	10500.	-204.553	---
700.	31.221	223.008	12053.	-205.790	---
750.	31.538	225.173	13622.	-207.010	---
(2 sigma)	---	---	---	---	---
800.	31.850	227.218	15207.	-208.210	---
850.	32.155	229.158	16807.	-209.386	---
900.	32.452	231.005	18422.	-210.536	---
950.	32.740	232.767	20052.	-211.660	---
1000.	33.019	234.453	21696.	-212.758	---
(2 sigma)	---	---	---	---	---
1050.	33.288	236.071	23354.	-213.830	---
1100.	33.548	237.626	25024.	-214.876	---
1150.	33.797	239.122	26708.	-215.898	---
1200.	34.037	240.566	28404.	-216.896	---
1250.	34.265	241.960	30112.	-217.871	---
(2 sigma)	---	---	---	---	---
1300.	34.483	243.308	31830.	-218.823	---
1350.	34.691	244.614	33560.	-219.754	---
1400.	34.887	245.879	35299.	-220.665	---
1450.	35.073	247.106	37048.	-221.556	---
1500.	35.248	248.298	38806.	-222.427	---
(2 sigma)	---	---	---	---	---
1550.	35.412	249.457	40573.	-223.281	---
1600.	35.564	250.583	42347.	-224.116	---
1650.	35.706	251.680	44129.	-224.935	---
1700.	35.837	252.748	45918.	-225.738	---
1750.	35.957	253.789	47713.	-226.524	---
(2 sigma)	---	---	---	---	---
1800.	36.065	254.803	49513.	-227.296	---
(2 sigma)	---	---	---	---	---

Table 43. Thermochemical properties of carbon monoxide (CO, ideal gas) at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-111296.	-128552.	33.574	0.	0.	0.
250.	-110888.	-132915.	27.771	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
273.15	-110722.	-134962.	25.809	0.	0.	0.
298.15	-110564.	-137188.	24.035	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
300.	-110553.	-137353.	23.915	0.	0.	0.
350.	-110310.	-141840.	21.168	0.	0.	0.
400.	-110155.	-146356.	19.112	0.	0.	0.
450.	-110077.	-150886.	17.514	0.	0.	0.
500.	-110067.	-155422.	16.237	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
550.	-110114.	-159955.	15.191	0.	0.	0.
600.	-110211.	-164482.	14.319	0.	0.	0.
650.	-110348.	-169000.	13.581	0.	0.	0.
700.	-110521.	-173505.	12.947	0.	0.	0.
750.	-110723.	-177997.	12.397	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
800.	-110951.	-182475.	11.914	0.	0.	0.
850.	-111199.	-186938.	11.488	0.	0.	0.
900.	-111465.	-191385.	11.108	0.	0.	0.
950.	-111745.	-195818.	10.767	0.	0.	0.
1000.	-112038.	-200235.	10.459	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
1050.	-112340.	-204637.	10.180	0.	0.	0.
1100.	-112651.	-209025.	9.926	0.	0.	0.
1150.	-112968.	-213399.	9.693	0.	0.	0.
1200.	-113290.	-217759.	9.479	0.	0.	0.
1250.	-113617.	-222105.	9.281	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
1300.	-113946.	-226438.	9.098	0.	0.	0.
1350.	-114278.	-230758.	8.929	0.	0.	0.
1400.	-114611.	-235066.	8.770	0.	0.	0.
1450.	-114946.	-239362.	8.623	0.	0.	0.
1500.	-115281.	-243647.	8.485	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
1550.	-115616.	-247920.	8.355	0.	0.	0.
1600.	-115951.	-252182.	8.233	0.	0.	0.
1650.	-116286.	-256435.	8.118	0.	0.	0.
1700.	-116620.	-260676.	8.010	0.	0.	0.
1750.	-116955.	-264909.	7.907	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
1800.	-117288.	-269131.	7.810	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.

Table 44. Thermophysical values for carbon dioxide (CO_2, ideal gas) at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	33.619	199.689	-3452.	-216.950	---
250.	35.115	207.329	-1739.	-214.284	---
(2 sigma)	---	---	---	---	---
273.15	36.066	210.480	-915.	-213.830	---
298.15	37.138	213.685	0.	-213.685	---
(2 sigma)	---	---	---	---	---
300.	37.218	213.915	69.	-213.685	---
350.	39.334	219.812	1983.	-214.146	---
400.	41.298	225.195	4000.	-215.196	---
450.	43.075	230.163	6110.	-216.586	---
500.	44.670	234.786	8304.	-218.178	---
(2 sigma)	---	---	---	---	---
550.	46.100	239.111	10574.	-219.886	---
600.	47.386	243.179	12912.	-221.659	---
650.	48.545	247.018	15310.	-223.464	---
700.	49.595	250.655	17764.	-225.277	---
750.	50.548	254.110	20268.	-227.085	---
(2 sigma)	---	---	---	---	---
800.	51.417	257.400	22818.	-228.878	---
850.	52.211	260.541	25409.	-230.649	---
900.	52.940	263.547	28038.	-232.394	---
950.	53.610	266.427	30702.	-234.110	---
1000.	54.228	269.193	33398.	-235.795	---
(2 sigma)	---	---	---	---	---
1050.	54.798	271.853	36124.	-237.449	---
1100.	55.326	274.414	38877.	-239.071	---
1150.	55.816	276.884	41656.	-240.662	---
1200.	56.270	279.270	44458.	-242.221	---
1250.	56.692	281.575	47282.	-243.750	---
(2 sigma)	---	---	---	---	---
1300.	57.085	283.807	50127.	-245.248	---
1350.	57.450	285.968	52990.	-246.716	---
1400.	57.791	288.064	55871.	-248.155	---
1450.	58.108	290.097	58769.	-249.567	---
1500.	58.403	292.072	61682.	-250.951	---
(2 sigma)	---	---	---	---	---
1550.	58.678	293.992	64609.	-252.309	---
1600.	58.934	295.859	67549.	-253.640	---
1650.	59.173	297.676	70502.	-254.947	---
1700.	59.394	299.446	73466.	-256.230	---
1750.	59.600	301.170	76441.	-257.490	---
(2 sigma)	---	---	---	---	---
1800.	59.791	302.852	79426.	-258.727	---
(2 sigma)	---	---	---	---	---

Table 45. Thermochemical properties of carbon dioxide (CO_2, ideal gas) at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-393507.	-394191.	102.952	0.	0.	0.
250.	-393583.	-394352.	82.395	0.	0.	0.
(? sigma)	---	---	---	0.	0.	0.
273.15	-393605.	-394422.	75.426	0.	0.	0.
298.15	-393626.	-394496.	69.114	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
300.	-393627.	-394502.	68.689	0.	0.	0.
350.	-393665.	-394644.	58.897	0.	0.	0.
400.	-393709.	-394781.	51.553	0.	0.	0.
450.	-393760.	-394912.	45.840	0.	0.	0.
500.	-393821.	-395037.	41.269	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
550.	-393891.	-395156.	37.529	0.	0.	0.
600.	-393969.	-395267.	34.411	0.	0.	0.
650.	-394053.	-395372.	31.772	0.	0.	0.
700.	-394143.	-395470.	29.510	0.	0.	0.
750.	-394238.	-395562.	27.549	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
800.	-394337.	-395647.	25.833	0.	0.	0.
850.	-394438.	-395725.	24.318	0.	0.	0.
900.	-394542.	-395798.	22.972	0.	0.	0.
950.	-394647.	-395865.	21.766	0.	0.	0.
1000.	-394753.	-395927.	20.681	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
1050.	-394859.	-395983.	19.699	0.	0.	0.
1100.	-394965.	-396034.	18.806	0.	0.	0.
1150.	-395070.	-396080.	17.991	0.	0.	0.
1200.	-395173.	-396122.	17.243	0.	0.	0.
1250.	-395276.	-396159.	16.555	0.	0.	0.
(? sigma)	---	---	---	0.	0.	0.
1300.	-395377.	-396192.	15.919	0.	0.	0.
1350.	-395475.	-396222.	15.331	0.	0.	0.
1400.	-395571.	-396248.	14.784	0.	0.	0.
1450.	-395665.	-396270.	14.275	0.	0.	0.
1500.	-395756.	-396290.	13.800	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
1550.	-395845.	-396306.	13.355	0.	0.	0.
1600.	-395930.	-396319.	12.938	0.	0.	0.
1650.	-396012.	-396330.	12.547	0.	0.	0.
1700.	-396091.	-396339.	12.178	0.	0.	0.
1750.	-396166.	-396345.	11.830	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
1800.	-396238.	-396349.	11.502	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.

Table 46. Thermophysical values for stable phases of the element calcium (Ca) at 1.01325 bars (1 atm). The sources of data are given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
	calcium (crystal, face centered cubic)				
200.	24.567	31.642	-2454.	-43.913	---
250.	25.033	37.181	-1213.	-42.032	---
(2 sigma)	---	---	---	---	---
273.15	25.180	39.404	-631.	-41.716	---
298.15	25.341	41.616	0.	-41.616	---
(2 sigma)	---	---	---	---	---
300.	25.354	41.773	47.	-41.617	---
350.	25.743	45.709	1324.	-41.927	---
400.	26.255	49.178	2623.	-42.620	---
450.	26.900	52.307	3952.	-43.525	---
500.	27.671	55.180	5315.	-44.549	---
(2 sigma)	---	---	---	---	---
550.	28.560	57.858	6721.	-45.639	---
600.	29.558	60.385	8173.	-46.763	---
650.	30.657	62.794	9678.	-47.904	---
700.	31.849	65.109	11240.	-49.051	---
720.	32.351	66.013	11882.	-49.510	---
	calcium (crystal, body centered cubic)				
720.	29.341	67.289	12801.	-49.510	---
750.	30.581	68.512	13700.	-50.245	---
(2 sigma)	---	---	---	---	---
800.	32.647	70.552	15281.	-51.451	---
850.	34.712	72.593	16965.	-52.634	---
900.	36.776	74.635	18752.	-53.800	---
950.	38.840	76.679	20642.	-54.950	---
1000.	40.903	78.724	22636.	-56.088	---
(2 sigma)	---	---	---	---	---
1050.	42.966	80.769	24733.	-57.214	---
1100.	45.029	82.816	26933.	-58.331	---
1112.	45.524	83.307	27476.	-58.598	---
	calcium (liquid)				
1112.	29.275	90.968	35995.	-58.598	---
1150.	29.275	91.952	37108.	-59.684	---
1200.	29.275	93.198	38571.	-61.055	---
1250.	29.275	94.393	40035.	-62.365	---
(2 sigma)	---	---	---	---	---
1300.	29.275	95.541	41499.	-63.619	---
1350.	29.275	96.646	42963.	-64.822	---
1400.	29.275	97.711	44427.	-65.977	---
1450.	29.275	98.738	45890.	-67.089	---
1500.	29.275	99.730	47354.	-68.161	---
(2 sigma)	---	---	---	---	---
1550.	29.275	100.690	48818.	-69.195	---
1600.	29.275	101.620	50282.	-70.194	---
1650.	29.275	102.521	51745.	-71.160	---
1700.	29.275	103.395	53209.	-72.095	---
1750.	29.275	104.243	54673.	-73.002	---
(2 sigma)	---	---	---	---	---
1755.	29.275	104.327	54819.	-73.091	---
	calcium (ideal monatomic gas)				
1755.	20.851	191.628	208032.	-73.091	---
1800.	20.862	192.156	208971.	-76.061	---
(2 sigma)	---	---	---	---	---

Table 47. Thermochemical properties of stable phases of the element calcium (Ca) at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
	calcium (crystal, face centered cubic)					
200.	0.	0.	0.	---	---	---
250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
273.15	0.	0.	0.	---	---	---
298.15	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
300.	0.	0.	0.	---	---	---
350.	0.	0.	0.	---	---	---
400.	0.	0.	0.	---	---	---
450.	0.	0.	0.	---	---	---
500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
550.	0.	0.	0.	---	---	---
600.	0.	0.	0.	---	---	---
650.	0.	0.	0.	---	---	---
700.	0.	0.	0.	---	---	---
720.	0.	0.	0.	---	---	---
	calcium (crystal, body centered cubic)					
720.	0.	0.	0.	---	---	---
750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
800.	0.	0.	0.	---	---	---
850.	0.	0.	0.	---	---	---
900.	0.	0.	0.	---	---	---
950.	0.	0.	0.	---	---	---
1000.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1050.	0.	0.	0.	---	---	---
1100.	0.	0.	0.	---	---	---
1112.	0.	0.	0.	---	---	---
	calcium (liquid)					
1112.	0.	0.	0.	---	---	---
1150.	0.	0.	0.	---	---	---
1200.	0.	0.	0.	---	---	---
1250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1300.	0.	0.	0.	---	---	---
1350.	0.	0.	0.	---	---	---
1400.	0.	0.	0.	---	---	---
1450.	0.	0.	0.	---	---	---
1500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1550.	0.	0.	0.	---	---	---
1600.	0.	0.	0.	---	---	---
1650.	0.	0.	0.	---	---	---
1700.	0.	0.	0.	---	---	---
1750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1755.	0.	0.	0.	---	---	---
	calcium (ideal diatomic gas)					
1755.	0.	0.	0.	---	---	---
1800.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---

Table 48. Thermophysical values for Ca-Al clinopyroxene, $CaAl_2SiO_6$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	99.917	88.557	-13535.	-156.232	63.4567
250.	140.960	115.672	-7421.	-145.357	63.5153
(2 sigma)	6.530	4.185	210.	4.100	0.0948
273.15	154.072	128.747	-4001.	-143.395	63.5443
298.15	165.638	142.756	0.	-142.756	63.5770
(2 sigma)	2.880	4.102	0.	4.102	0.0725
300.	166.408	143.783	307.	-142.759	63.5794
350.	183.831	170.819	9088.	-144.854	63.6483
400.	196.596	196.240	18613.	-149.706	63.7212
450.	206.414	219.986	28699.	-156.211	63.7974
500.	214.247	242.153	39222.	-163.709	63.8765
(2 sigma)	2.171	3.913	381.	4.050	0.0431
550.	220.673	262.884	50100.	-171.793	63.9581
600.	226.063	282.323	61272.	-180.203	64.0417
650.	230.668	300.604	72693.	-188.768	64.1270
700.	234.659	317.848	84329.	-197.378	64.2138
750.	238.162	334.159	96151.	-205.958	64.3018
(2 sigma)	1.777	3.784	763.	3.946	0.0461
800.	241.268	349.631	108138.	-214.458	64.3909
850.	244.047	364.343	120272.	-222.846	64.4808
900.	246.553	378.364	132538.	-231.099	64.5716
950.	248.828	391.757	144924.	-239.205	64.6629
1000.	250.906	404.573	157418.	-247.156	64.7548
(2 sigma)	2.782	3.678	1051.	3.858	0.0379
1050.	252.814	416.862	170012.	-254.946	64.8472
1100.	254.573	428.664	182697.	-262.576	64.9399
1150.	256.203	440.017	195467.	-270.046	65.0330
1200.	257.718	450.953	208315.	-277.357	65.1264
1250.	259.131	461.502	221237.	-284.513	65.2200
(2 sigma)	4.066	3.675	1592.	3.786	0.0404
1300.	260.454	471.692	234227.	-291.517	65.3138
1350.	261.696	481.545	247281.	-298.374	65.4077
1400.	262.865	491.084	260395.	-305.087	65.5018
1450.	263.967	500.327	273566.	-311.661	65.5960
1500.	265.009	509.294	286791.	-318.100	65.6904
(2 sigma)	5.196	3.849	2536.	3.731	0.0652
1550.	265.996	518.000	300066.	-324.409	65.7848
1600.	266.933	526.460	313390.	-330.591	65.8792
1650.	267.825	534.687	326759.	-336.652	65.9738
1700.	268.673	542.695	340171.	-342.595	66.0684
1750.	269.483	550.495	353625.	-348.424	66.1630
(2 sigma)	6.149	4.201	3821.	3.700	0.0997
1800.	270.257	558.098	367119.	-354.143	66.2577
(2 sigma)	6.321	4.290	4112.	3.698	0.1071

Table 49. Thermochemical properties of Ca-Al clinopyroxene, $CaAl_2SiO_6$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-3294801.	-3180161.	830.572	-76525.	-79495.	20.762
250.	-3297395.	-3151165.	658.399	-77018.	-80168.	16.750
(2 sigma)	---	---	---	5449.	4502.	0.941
273.15	-3298105.	-3137591.	600.003	-77095.	-80456.	15.386
298.15	-3298625.	-3122875.	547.114	-77123.	-80762.	14.149
(2 sigma)	---	---	---	5447.	4324.	0.758
300.	-3298655.	-3121784.	543.551	-77123.	-80785.	14.066
350.	-3299095.	-3092262.	461.495	-77086.	-81397.	12.148
400.	-3299000.	-3062716.	399.949	-77009.	-82018.	10.710
450.	-3298543.	-3033205.	352.085	-76942.	-82648.	9.594
500.	-3297841.	-3003758.	313.800	-76906.	-83284.	8.701
(2 sigma)	---	---	---	5418.	3601.	0.376
550.	-3296977.	-2974391.	282.484	-76912.	-83922.	7.970
600.	-3296012.	-2945107.	256.394	-76965.	-84558.	7.361
650.	-3294996.	-2915906.	234.325	-77067.	-85186.	6.846
700.	-3293969.	-2886783.	215.414	-77218.	-85806.	6.403
750.	-3293797.	-2857698.	199.028	-77416.	-86412.	6.018
(2 sigma)	---	---	---	5377.	2764.	0.192
800.	-3292730.	-2828660.	184.692	-77663.	-87004.	5.681
850.	-3291769.	-2799685.	172.048	-78668.	-87574.	5.382
900.	-3290933.	-2770764.	160.811	-78584.	-88101.	5.113
950.	-3311497.	-2741238.	150.724	-78479.	-88632.	4.873
1000.	-3310685.	-2711246.	141.621	-78357.	-89170.	4.658
(2 sigma)	---	---	---	5342.	2021.	0.106
1050.	-3309924.	-2681292.	133.387	-78219.	-89713.	4.463
1100.	-3309218.	-2651374.	125.903	-78069.	-90264.	4.286
1150.	-3316443.	-2621207.	119.059	-77908.	-90822.	4.125
1200.	-3314916.	-2591012.	112.784	-77738.	-91387.	3.978
1250.	-3313351.	-2560881.	107.013	-77563.	-91960.	3.843
(2 sigma)	---	---	---	5393.	1461.	0.061
1300.	-3311751.	-2530814.	101.689	-77384.	-92539.	3.718
1350.	-3310117.	-2500809.	96.762	-77203.	-93125.	3.603
1400.	-3308450.	-2470865.	92.189	-77023.	-93718.	3.497
1450.	-3306753.	-2440981.	87.934	-76847.	-94318.	3.398
1500.	-3305026.	-2411156.	83.964	-76676.	-94923.	3.306
(2 sigma)	---	---	---	5669.	1333.	0.046
1550.	-3303270.	-2381389.	80.252	-76513.	-95534.	3.219
1600.	-3301485.	-2351679.	76.774	-76360.	-96150.	3.139
1650.	-3299672.	-2322026.	73.509	-76220.	-96771.	3.064
1700.	-3348341.	-2291978.	70.424	-76096.	-97395.	2.993
1750.	-3346330.	-2260938.	67.485	-75989.	-98023.	2.926
(2 sigma)	---	---	---	6284.	1804.	0.054
1800.	-3497121.	-2226032.	64.598	-75902.	-98654.	2.863
(2 sigma)	---	---	---	6453.	1952.	0.057

Table 50. Thermophysical values for anorthite, $CaAl_2Si_2O_8$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T	C_p°	S°	$H_T^\circ - H_{298}^\circ$	$[G_T^\circ - H_{298}^\circ]/T$	V°
K	J/(mol K)	J/(mol K)	J/mol	J/(mol K)	cm^3/mol
200.	158.036	125.573	-18292.	-217.033	100.6014
250.	187.683	164.097	-9632.	-202.626	100.6655
(2 sigma)	0.200	0.155	9.	0.152	0.0812
273.15	199.792	181.255	-5145.	-200.091	100.6951
298.15	211.605	199.271	0.	-199.271	100.7272
(2 sigma)	0.154	0.152	0.	0.152	0.0763
300.	212.428	200.582	392.	-199.275	100.7296
350.	232.271	234.876	11528.	-201.938	100.7936
400.	248.088	266.964	23552.	-208.083	100.8577
450.	260.749	296.943	36285.	-216.310	100.9218
500.	270.967	324.963	49587.	-225.790	100.9859
(2 sigma)	0.427	0.188	47.	0.153	0.0613
550.	279.295	351.193	63350.	-236.011	101.0500
600.	286.166	375.798	77492.	-246.645	101.1141
650.	291.914	398.937	91948.	-257.479	101.1782
700.	296.803	420.754	106669.	-268.370	101.2423
750.	301.042	441.379	121617.	-279.222	101.3064
(2 sigma)	0.750	0.340	175.	0.170	0.0615
800.	304.801	460.930	136765.	-289.973	101.3704
850.	308.215	479.512	152092.	-300.581	101.4345
900.	311.397	497.220	167583.	-311.017	101.4986
950.	314.440	514.139	183229.	-321.266	101.5627
1000.	317.423	530.343	199026.	-331.317	101.6268
(2 sigma)	1.217	0.491	339.	0.212	0.0815
1050.	320.409	545.902	214971.	-341.168	101.6909
1100.	323.456	560.878	231068.	-350.816	101.7550
1150.	326.611	575.325	247319.	-360.265	101.8191
1200.	329.914	589.295	263731.	-369.519	101.8831
1250.	333.402	602.833	280313.	-378.582	101.9472
(2 sigma)	3.451	0.698	676.	0.260	0.1112
1300.	337.105	615.980	297075.	-387.461	102.0113
1350.	341.050	628.776	314028.	-396.163	102.0754
1400.	345.260	641.254	331185.	-404.694	102.1395
1450.	349.757	653.448	348559.	-413.062	102.2036
1500.	354.560	665.385	366165.	-421.275	102.2677
(2 sigma)	7.990	1.450	1881.	0.328	0.1446
1550.	359.684	677.094	384020.	-429.339	102.3318
1600.	365.145	688.598	402139.	-437.261	102.3958
1650.	370.956	699.923	420540.	-445.050	102.4599
1700.	377.128	711.087	439241.	-452.710	102.5240
1750.	383.673	722.113	458259.	-460.250	102.5881
(2 sigma)	14.878	3.035	4581.	0.517	0.1798
1800.	390.600	733.018	477615.	-467.676	102.6522
(2 sigma)	16.544	3.458	5349.	0.580	0.1869

Table 51. Thermochemical properties of anorthite, $CaAl_2Si_2O_8$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-4226995.	-4078749.	1065.259	-98839.	-104007.	27.164
250.	-4229349.	-4041394.	844.402	-98598.	-105334.	22.008
(2 sigma)	---	---	---	1167.	1166.	0.244
273.15	-4230100.	-4023954.	769.503	-98554.	-105960.	20.263
298.15	-4230697.	-4005058.	701.669	-98525.	-106639.	18.683
(2 sigma)	---	---	---	1167.	1165.	0.204
300.	-4230733.	-4003658.	697.098	-98524.	-106689.	18.576
350.	-4231330.	-3965755.	591.856	-98490.	-108053.	16.126
400.	-4231326.	-3927810.	512.919	-98480.	-109420.	14.289
450.	-4230876.	-3889894.	451.527	-98507.	-110787.	12.860
500.	-4230107.	-3852046.	402.420	-98591.	-112147.	11.716
(2 sigma)	---	---	---	1168.	1165.	0.122
550.	-4229118.	-3814286.	362.250	-98753.	-113496.	10.779
600.	-4227990.	-3776623.	328.784	-99007.	-114825.	9.996
650.	-4226786.	-3739057.	300.474	-99367.	-116130.	9.332
700.	-4225557.	-3701586.	276.216	-99838.	-117402.	8.761
750.	-4225177.	-3664166.	255.195	-100425.	-118637.	8.263
(2 sigma)	---	---	---	1174.	1168.	0.081
800.	-4223897.	-3626807.	236.806	-101126.	-119829.	7.824
850.	-4222721.	-3589526.	220.585	-103365.	-120963.	7.433
900.	-4221665.	-3552310.	206.171	-103441.	-121996.	7.080
950.	-4241996.	-3514502.	193.241	-103485.	-123025.	6.764
1000.	-4240934.	-3476241.	181.580	-103496.	-124053.	6.480
(2 sigma)	---	---	---	1208.	1181.	0.062
1050.	-4239895.	-3438032.	171.033	-103466.	-125082.	6.222
1100.	-4238871.	-3399872.	161.446	-103390.	-126113.	5.989
1150.	-4245728.	-3361478.	152.683	-103258.	-127148.	5.775
1200.	-4243767.	-3323074.	144.650	-103060.	-128191.	5.580
1250.	-4241688.	-3284754.	137.262	-102785.	-129244.	5.401
(2 sigma)	---	---	---	1372.	1204.	0.050
1300.	-4239479.	-3246519.	130.447	-102420.	-130309.	5.236
1350.	-4237123.	-3208373.	124.139	-101951.	-131390.	5.084
1400.	-4234604.	-3170317.	118.286	-101365.	-132491.	4.943
1450.	-4231907.	-3132353.	112.839	-100646.	-133615.	4.813
1500.	-4229012.	-3094487.	107.760	-99779.	-134766.	4.693
(2 sigma)	---	---	---	2285.	1245.	0.043
1550.	-4225902.	-3056720.	103.011	-98748.	-135948.	4.581
1600.	-4222556.	-3019057.	98.562	-97536.	-137167.	4.478
1650.	-4218956.	-2981503.	94.386	-96125.	-138427.	4.382
1700.	-4316099.	-2943162.	90.432	-94499.	-139733.	4.293
1750.	-4311643.	-2902845.	86.645	-92639.	-141090.	4.211
(2 sigma)	---	---	---	4817.	1424.	0.043
1800.	-4459694.	-2858737.	82.958	-90528.	-142503.	4.135
(2 sigma)	---	---	---	5565.	1505.	0.044

Table 52. Thermophysical values for margarite, $CaAl_4Si_2O_{10}(OH)_2$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	233.508	150.974	-28011.	-291.027	133.4726
250.	288.597	209.347	-14880.	-268.866	133.6249
(2 sigma)	0.520	0.686	28.	0.678	0.2834
273.15	308.720	235.803	-7961.	-264.947	133.6954
298.15	327.702	263.677	0.	-263.677	133.7715
(2 sigma)	0.727	0.678	0.	0.678	0.2567
300.	329.009	265.708	607.	-263.684	133.7772
350.	360.200	318.863	17869.	-267.810	133.9295
400.	385.154	368.648	36524.	-277.338	134.0818
450.	405.658	415.234	56310.	-290.100	134.2341
500.	422.853	458.889	77035.	-304.819	134.3864
(2 sigma)	1.435	0.883	228.	0.687	0.5331
550.	437.512	499.897	98553.	-320.709	134.5387
600.	450.173	538.521	120753.	-337.266	134.6910
650.	461.230	575.000	143544.	-354.163	134.8433
700.	470.973	609.545	166854.	-371.182	134.9956
750.	479.627	642.339	190623.	-388.175	135.1479
(2 sigma)	2.107	1.370	626.	0.770	1.0854
800.	487.363	673.545	214802.	-405.044	135.3002
850.	494.320	703.304	239347.	-421.720	135.4525
900.	500.606	731.739	264222.	-438.159	135.6048
950.	506.312	758.961	289398.	-454.332	135.7571
1000.	511.510	785.066	314845.	-470.221	135.9094
(2 sigma)	3.359	1.914	1201.	0.928	1.6620
1050.	516.262	810.139	340541.	-485.814	136.0617
1100.	520.620	834.258	366465.	-501.108	136.2140
1150.	524.626	857.490	392597.	-516.101	136.3663
1200.	528.317	879.897	418922.	-530.795	136.5186
1250.	531.726	901.534	445424.	-545.194	136.6709
(2 sigma)	5.013	2.597	2115.	1.134	2.2442

Table 53. Thermochemical properties of margarite, $CaAl_4Si_2O_{10}(OH)_2$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-6235930.	-5983852.	1562.821	---	---	---
250.	-6240331.	-5920281.	1236.974	---	---	---
(2 sigma)	---	---	---	---	---	---
273.15	-6241747.	-5890578.	1126.458	-148246.	-141167.	26.995
298.15	-6242914.	-5858382.	1026.364	-149196.	-140477.	24.611
(2 sigma)	---	---	---	1692.	1636.	0.287
300.	-6242987.	-5855996.	1019.619	-149265.	-140423.	24.450
350.	-6244341.	-5791375.	864.315	-151076.	-138805.	20.715
400.	-6244706.	-5726630.	747.821	-192566.	-134031.	17.503
450.	-6244310.	-5661888.	657.214	-192183.	-126736.	14.711
500.	-6243327.	-5597222.	584.737	-191764.	-119487.	12.483
(2 sigma)	---	---	---	1757.	1599.	0.167
550.	-6241893.	-5532678.	525.450	-191321.	-112280.	10.663
600.	-6240120.	-5468280.	476.056	-190866.	-105115.	9.151
650.	-6238101.	-5404040.	434.274	-190410.	-97987.	7.874
700.	-6235913.	-5339963.	398.473	-189962.	-90895.	6.783
750.	-6234459.	-5276009.	367.454	-189531.	-83834.	5.839
(2 sigma)	---	---	---	1929.	1553.	0.108
800.	-6232018.	-5212192.	340.321	-189124.	-76801.	5.015
850.	-6229620.	-5148527.	316.390	-190174.	-69782.	4.288
900.	-6227308.	-5085001.	295.126	-188992.	-62733.	3.641
950.	-6267639.	-5020305.	276.035	-187724.	-55753.	3.066
1000.	-6265070.	-4954722.	258.808	-186382.	-48842.	2.551
(2 sigma)	---	---	---	2249.	1574.	0.082
1050.	-6262458.	-4889269.	243.228	-184978.	-41999.	2.089
1100.	-6259817.	-4823940.	229.070	-183521.	-35224.	1.673
1150.	-6265034.	-4758452.	216.136	-182021.	-28517.	1.295
1200.	-6261432.	-4693026.	204.282	-180487.	-21876.	0.952
1250.	-6257733.	-4627751.	193.383	-178928.	-15299.	0.639
(2 sigma)	---	---	---	2885.	1760.	0.074

Table 54. Thermophysical values for calcite, $CaCO_3$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	65.922	61.997	-7378.	-98.884	36.7652
250.	75.672	77.806	-3826.	-93.110	36.7709
(2 sigma)	0.251	0.446	10.	0.444	0.1402
273.15	79.387	84.673	-2031.	-92.106	36.7739
298.15	82.991	91.783	0.	-91.783	36.7775
(2 sigma)	0.163	0.444	0.	0.444	0.1407
300.	83.244	92.297	154.	-91.785	36.7777
350.	89.447	105.609	4476.	-92.822	36.7854
400.	94.725	117.907	9083.	-95.199	36.7939
450.	99.342	129.336	13937.	-98.364	36.8029
500.	103.469	140.020	19009.	-102.001	36.8126
(2 sigma)	0.123	0.448	25.	0.444	0.1487
550.	107.218	150.060	24278.	-105.918	36.8226
600.	110.672	159.539	29726.	-109.995	36.8331
650.	113.887	168.526	35341.	-114.155	36.8439
700.	116.908	177.077	41112.	-118.347	36.8550
750.	119.767	185.242	47029.	-122.536	36.8663
(2 sigma)	0.203	0.451	43.	0.445	0.1416
800.	122.489	193.059	53086.	-126.701	36.8778
850.	125.096	200.563	59276.	-130.827	36.8894
900.	127.603	207.785	65594.	-134.903	36.9013
950.	130.025	214.749	72035.	-138.923	36.9132
1000.	132.371	221.479	78595.	-142.884	36.9252
(2 sigma)	0.545	0.461	103.	0.446	0.1517
1050.	134.650	227.993	85271.	-146.782	36.9374
1100.	136.872	234.308	92059.	-150.618	36.9496
1150.	139.041	240.440	98957.	-154.390	36.9618
1200.	141.163	246.403	105963.	-158.101	36.9741
1250.	143.243	252.208	113073.	-161.749	36.9865
(2 sigma)	0.969	0.517	279.	0.448	0.2026
1300.	145.286	257.866	120286.	-165.338	36.9989
1350.	147.294	263.387	127601.	-168.867	37.0113
1400.	149.271	268.779	135015.	-172.340	37.0238
1450.	151.219	274.051	142527.	-175.756	37.0362
1500.	153.142	279.210	150137.	-179.119	37.0487
(2 sigma)	1.434	0.647	573.	0.455	0.2805
1550.	155.040	284.263	157841.	-182.430	37.0612
1600.	156.916	289.215	165640.	-185.690	37.0738
1650.	158.772	294.072	173533.	-188.901	37.0863
1700.	160.609	298.839	181517.	-192.064	37.0989
1750.	162.428	303.521	189593.	-195.182	37.1114
(2 sigma)	1.923	0.848	989.	0.474	0.3705
1800.	164.231	308.122	197760.	-198.255	37.1240
(2 sigma)	2.023	0.895	1087.	0.480	0.3893

Table 55. Thermochemical properties of calcite, $CaCO_3$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

T	Formation from the Elements			Formation from the Oxides		
	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-1208980.	-1156457.	302.035	-180485.	-148379.	38.752
250.	-1209187.	-1143294.	238.878	-180470.	-140351.	29.325
(2 sigma)	---	---	---	894.	826.	0.173
273.15	-1209155.	-1137193.	217.466	-180419.	-136638.	26.129
298.15	-1209058.	-1130610.	198.078	-180338.	-132634.	23.237
(2 sigma)	---	---	---	894.	814.	0.143
300.	-1209048.	-1130124.	196.772	-180332.	-132338.	23.042
350.	-1208696.	-1116995.	166.702	-180099.	-124356.	18.559
400.	-1208200.	-1103927.	144.158	-179785.	-116413.	15.202
450.	-1207600.	-1090928.	126.632	-179396.	-108515.	12.596
500.	-1206923.	-1078000.	112.618	-178933.	-100663.	10.516
(2 sigma)	---	---	---	895.	768.	0.080
550.	-1206187.	-1065143.	101.159	-178398.	-92861.	8.819
600.	-1205405.	-1052355.	91.616	-177792.	-85112.	7.410
650.	-1204587.	-1039634.	83.546	-177114.	-77415.	6.221
700.	-1203741.	-1026977.	76.634	-176365.	-69774.	5.207
750.	-1203709.	-1014345.	70.645	-175545.	-62188.	4.331
(2 sigma)	---	---	---	898.	722.	0.050
800.	-1202717.	-1001753.	65.408	-174652.	-54660.	3.569
850.	-1201748.	-989223.	60.790	-173689.	-47189.	2.900
900.	-1200801.	-976749.	56.689	-172653.	-39778.	2.309
950.	-1199879.	-964327.	53.022	-171546.	-32426.	1.783
1000.	-1198979.	-951952.	49.725	-170367.	-25134.	1.313
(2 sigma)	---	---	---	910.	689.	0.036
1050.	-1198104.	-939623.	46.744	-169116.	-17903.	0.891
1100.	-1197252.	-927334.	44.035	-167793.	-10733.	0.510
1150.	-1204295.	-914803.	41.552	-166399.	-3625.	0.165
1200.	-1202548.	-902254.	39.274	-164933.	3421.	-0.149
1250.	-1200721.	-889779.	37.182	-163396.	10405.	-0.435
(2 sigma)	---	---	---	958.	673.	0.028
1300.	-1198813.	-877379.	35.253	-161787.	17325.	-0.696
1350.	-1196826.	-865053.	33.471	-160108.	24183.	-0.936
1400.	-1194757.	-852803.	31.818	-158358.	30976.	-1.156
1450.	-1192608.	-840628.	30.283	-156537.	37706.	-1.358
1500.	-1190377.	-828529.	28.852	-154645.	44372.	-1.545
(2 sigma)	---	---	---	1096.	680.	0.024
1550.	-1188065.	-816505.	27.516	-152684.	50974.	-1.718
1600.	-1185672.	-804557.	26.266	-150652.	57512.	-1.878
1650.	-1183196.	-792685.	25.094	-148551.	63984.	-2.026
1700.	-1180638.	-780890.	23.994	-146380.	70392.	-2.163
1750.	-1177997.	-769171.	22.958	-144140.	76736.	-2.290
(2 sigma)	---	---	---	1376.	731.	0.022
1800.	-1328108.	-753605.	21.869	-141831.	83014.	-2.409
(2 sigma)	---	---	---	1452.	749.	0.022

Table 56. Thermophysical values for aragonite, $CaCO_3$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	66.274	58.305	-7338.	-94.993	34.1417
250.	75.230	74.104	-3789.	-89.261	34.1420
(2 sigma)	0.249	0.429	13.	0.430	0.0876
273.15	78.628	80.917	-2008.	-88.267	34.1423
298.15	81.915	87.948	0.	-87.948	34.1426
(2 sigma)	0.325	0.430	0.	0.430	0.0876
300.	82.145	88.455	152.	-87.949	34.1426
350.	87.777	101.554	4404.	-88.971	34.1434
400.	92.542	113.594	8915.	-91.306	34.1443
450.	96.688	124.739	13648.	-94.410	34.1454
500.	100.373	135.120	18576.	-97.967	34.1466
(2 sigma)	0.678	0.440	80.	0.428	0.0876
550.	103.706	144.845	23680.	-101.792	34.1478
600.	106.761	154.002	28942.	-105.765	34.1492
650.	109.593	162.660	34352.	-109.811	34.1506
700.	112.242	170.880	39898.	-113.882	34.1521
750.	114.740	178.710	45574.	-117.945	34.1536
(2 sigma)	2.367	0.654	396.	0.413	0.0877
800.	117.110	186.191	51370.	-121.978	34.1552
850.	119.371	193.359	57283.	-125.968	34.1568
900.	121.540	200.244	63306.	-129.904	34.1585
950.	123.627	206.872	69435.	-133.782	34.1602
1000.	125.644	213.265	75667.	-137.597	34.1619
(2 sigma)	4.607	1.495	1235.	0.461	0.0884
1050.	127.599	219.442	81999.	-141.348	34.1636
1100.	129.499	225.422	88426.	-145.035	34.1653
1150.	131.350	231.220	94948.	-148.656	34.1670
1200.	133.158	236.848	101561.	-152.214	34.1688
1250.	134.926	242.320	108263.	-155.710	34.1706
(2 sigma)	7.075	2.733	2676.	0.702	0.0897
1300.	136.658	247.646	115053.	-159.144	34.1723
1350.	138.359	252.835	121928.	-162.518	34.1741
1400.	140.030	257.897	128888.	-165.834	34.1759
1450.	141.674	262.840	135931.	-169.095	34.1777
1500.	143.294	267.670	143055.	-172.300	34.1795
(2 sigma)	9.667	4.222	4755.	1.120	0.0917
1550.	144.892	272.395	150260.	-175.453	34.1813
1600.	146.469	277.020	157544.	-178.555	34.1831
1650.	148.026	281.551	164906.	-181.608	34.1849
1700.	149.566	285.993	172346.	-184.613	34.1867
1750.	151.089	290.351	179863.	-187.572	34.1885
(2 sigma)	12.336	5.893	7494.	1.659	0.0945
1800.	152.598	294.628	187455.	-190.486	34.1903
(2 sigma)	12.876	6.245	8123.	1.778	0.0951

Table 57. Thermochemical properties of aragonite, $CaCO_3$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-1209543.	-1156283.	301.990	-181049.	-148204.	38.707
250.	-1209753.	-1142935.	238.803	-181037.	-139992.	29.250
(2 sigma)	---	---	---	827.	797.	0.166
273.15	-1209736.	-1136748.	217.381	-180999.	-136192.	26.044
298.15	-1209661.	-1130070.	197.983	-180942.	-132094.	23.142
(2 sigma)	---	---	---	827.	792.	0.139
300.	-1209654.	-1129576.	196.677	-180937.	-131791.	22.947
350.	-1209371.	-1116251.	166.591	-180774.	-123612.	18.448
400.	-1208971.	-1102974.	144.034	-180557.	-115460.	15.078
450.	-1208492.	-1089752.	126.495	-180288.	-107339.	12.460
500.	-1207959.	-1076587.	112.470	-179969.	-99250.	10.369
(2 sigma)	---	---	---	837.	778.	0.081
550.	-1207388.	-1063477.	101.001	-179600.	-91195.	8.661
600.	-1206792.	-1050420.	91.447	-179179.	-83177.	7.241
650.	-1206179.	-1037414.	83.368	-178707.	-75195.	6.043
700.	-1205557.	-1024456.	76.446	-178182.	-67252.	5.018
750.	-1205768.	-1011505.	70.447	-177604.	-59348.	4.133
(2 sigma)	---	---	---	939.	763.	0.053
800.	-1205036.	-998578.	65.200	-176972.	-51485.	3.362
850.	-1204345.	-985696.	60.573	-176285.	-43663.	2.683
900.	-1203693.	-972853.	56.463	-175545.	-35883.	2.083
950.	-1203082.	-960046.	52.787	-174749.	-28145.	1.548
1000.	-1202511.	-947269.	49.480	-173898.	-20451.	1.068
(2 sigma)	---	---	---	1519.	783.	0.041
1050.	-1201980.	-934521.	46.490	-172991.	-12801.	0.637
1100.	-1201488.	-921796.	43.772	-172029.	-5195.	0.247
1150.	-1208908.	-908813.	41.280	-171012.	2366.	-0.107
1200.	-1207553.	-895794.	38.993	-169938.	9881.	-0.430
1250.	-1206134.	-882833.	36.892	-168809.	17351.	-0.725
(2 sigma)	---	---	---	2832.	1033.	0.043
1300.	-1204650.	-869930.	34.954	-167624.	24774.	-0.995
1350.	-1203102.	-857085.	33.163	-166384.	32151.	-1.244
1400.	-1201488.	-844299.	31.501	-165088.	39480.	-1.473
1450.	-1199808.	-831572.	29.956	-163737.	46763.	-1.685
1500.	-1198062.	-818904.	28.517	-162330.	53997.	-1.880
(2 sigma)	---	---	---	4855.	1731.	0.060
1550.	-1196250.	-806295.	27.172	-160868.	61184.	-2.062
1600.	-1194371.	-793745.	25.913	-159352.	68323.	-2.231
1650.	-1192426.	-781256.	24.732	-157780.	75414.	-2.387
1700.	-1190412.	-768826.	23.623	-156154.	82456.	-2.534
1750.	-1188331.	-756457.	22.579	-154474.	89450.	-2.670
(2 sigma)	---	---	---	7567.	2908.	0.087
1800.	-1339017.	-740224.	21.481	-152740.	96395.	-2.797
(2 sigma)	---	---	---	8192.	3200.	0.093

Table 58. Thermophysical values for lime, CaO, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	33.606	22.842	-3778.	-41.734	16.6616
250.	38.873	30.955	-1956.	-38.777	16.6978
(2 sigma)	---	---	---	---	---
273.15	40.605	34.475	-1035.	-38.265	16.7145
298.15	42.153	38.100	0.	-38.100	16.7326
(2 sigma)	---	---	---	---	---
300.	42.256	38.361	78.	-38.101	16.7339
350.	44.624	45.063	2253.	-38.625	16.7701
400.	46.380	51.142	4530.	-39.815	16.8062
450.	47.738	56.686	6885.	-41.387	16.8424
500.	48.821	61.774	9300.	-43.174	16.8785
(2 sigma)	---	---	---	---	---
550.	49.707	66.470	11764.	-45.081	16.9147
600.	50.446	70.827	14268.	-47.048	16.9508
650.	51.075	74.891	16806.	-49.035	16.9870
700.	51.617	78.696	19374.	-51.019	17.0231
750.	52.092	82.274	21967.	-52.985	17.0593
(2 sigma)	---	---	---	---	---
800.	52.513	85.649	24582.	-54.922	17.0954
850.	52.891	88.845	27218.	-56.824	17.1316
900.	53.235	91.878	29871.	-58.688	17.1677
950.	53.550	94.764	32541.	-60.511	17.2039
1000.	53.842	97.519	35225.	-62.293	17.2400
(2 sigma)	---	---	---	---	---
1050.	54.117	100.152	37924.	-64.034	17.2762
1100.	54.376	102.676	40637.	-65.733	17.3123
1150.	54.624	105.099	43362.	-67.393	17.3485
1200.	54.863	107.428	46099.	-69.012	17.3846
1250.	55.095	109.673	48848.	-70.594	17.4208
(2 sigma)	---	---	---	---	---
1300.	55.321	111.838	51608.	-72.139	17.4569
1350.	55.545	113.930	54380.	-73.648	17.4931
1400.	55.766	115.954	57163.	-75.123	17.5293
1450.	55.986	117.915	59957.	-76.565	17.5654
1500.	56.207	119.817	62762.	-77.976	17.6016
(2 sigma)	---	---	---	---	---
1550.	56.429	121.663	65577.	-79.355	17.6377
1600.	56.652	123.458	68404.	-80.705	17.6739
1650.	56.879	125.205	71243.	-82.028	17.7100
1700.	57.109	126.906	74092.	-83.323	17.7462
1750.	57.342	128.565	76954.	-84.592	17.7823
(2 sigma)	---	---	---	---	---
1800.	57.580	130.184	79827.	-85.836	17.8185
(2 sigma)	---	---	---	---	---

Table 59. Thermochemical properties of lime, CaO, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-634987.	-613888.	160.331	0.0	0.0	0.0
250.	-635133.	-608591.	127.158	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
273.15	-635131.	-606133.	115.911	0.0	0.0	0.0
298.15	-635094.	-603480.	105.727	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
300.	-635090.	-603284.	105.041	0.0	0.0	0.0
350.	-634931.	-597994.	89.246	0.0	0.0	0.0
400.	-634706.	-592732.	77.403	0.0	0.0	0.0
450.	-634444.	-587501.	68.195	0.0	0.0	0.0
500.	-634169.	-582300.	60.832	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
550.	-633898.	-577126.	54.811	0.0	0.0	0.0
600.	-633644.	-571977.	49.795	0.0	0.0	0.0
650.	-633419.	-566847.	45.552	0.0	0.0	0.0
700.	-633232.	-561733.	41.917	0.0	0.0	0.0
750.	-633927.	-556595.	38.765	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
800.	-633728.	-551447.	36.006	0.0	0.0	0.0
850.	-633621.	-546308.	33.572	0.0	0.0	0.0
900.	-633606.	-541173.	31.409	0.0	0.0	0.0
950.	-633686.	-536036.	29.473	0.0	0.0	0.0
1000.	-633860.	-530892.	27.731	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1050.	-634129.	-525737.	26.154	0.0	0.0	0.0
1100.	-634494.	-520568.	24.720	0.0	0.0	0.0
1150.	-642827.	-515099.	23.397	0.0	0.0	0.0
1200.	-642442.	-509554.	22.180	0.0	0.0	0.0
1250.	-642049.	-504025.	21.062	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1300.	-641649.	-498512.	20.030	0.0	0.0	0.0
1350.	-641242.	-493014.	19.076	0.0	0.0	0.0
1400.	-640828.	-487532.	18.190	0.0	0.0	0.0
1450.	-640406.	-482064.	17.366	0.0	0.0	0.0
1500.	-639976.	-476612.	16.597	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1550.	-639537.	-471173.	15.878	0.0	0.0	0.0
1600.	-639090.	-465749.	15.205	0.0	0.0	0.0
1650.	-638633.	-460339.	14.573	0.0	0.0	0.0
1700.	-638167.	-454944.	13.979	0.0	0.0	0.0
1750.	-637691.	-449562.	13.419	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1800.	-790039.	-440270.	12.776	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0

Table 60. Thermophysical values for stable phases with the composition $CaSiO_3$ at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
		wollastonite			
200.	65.696	50.950	-7572.	-88.810	39.5612
250.	77.862	66.995	-3965.	-82.857	39.6874
(2 sigma)	0.075	0.689	3.	0.689	0.1482
273.15	82.290	74.088	-2111.	-81.815	39.7403
298.15	86.456	81.479	0.	-81.479	39.7940
(2 sigma)	0.076	0.689	0.	0.689	0.0986
300.	86.742	82.015	160.	-81.481	39.7978
350.	93.556	95.919	4675.	-82.563	39.8948
400.	98.972	108.778	9493.	-85.047	39.9804
450.	103.389	120.699	14555.	-88.354	40.0564
500.	107.062	131.788	19819.	-92.149	40.1243
(2 sigma)	0.118	0.688	17.	0.688	0.0807
550.	110.165	142.141	25252.	-96.229	40.1854
600.	112.818	151.844	30828.	-100.463	40.2406
650.	115.108	160.967	36528.	-104.770	40.2909
700.	117.102	169.572	42334.	-109.094	40.3370
750.	118.849	177.712	48234.	-113.400	40.3795
(2 sigma)	0.180	0.690	50.	0.688	0.0745
800.	120.387	185.432	54216.	-117.663	40.4191
850.	121.748	192.772	60270.	-121.867	40.4562
900.	122.955	199.766	66388.	-126.002	40.4911
950.	124.029	206.443	72563.	-130.061	40.5242
1000.	124.987	212.830	78789.	-134.041	40.5558
(2 sigma)	0.260	0.693	80.	0.688	0.1827
1050.	125.842	218.949	85060.	-137.940	40.5860
1100.	126.605	224.821	91371.	-141.756	40.6152
1150.	127.286	230.464	97719.	-145.491	40.6434
1200.	127.894	235.895	104099.	-149.146	40.6709
1250.	128.435	241.127	110507.	-152.721	40.6977
(2 sigma)	0.837	0.696	145.	0.688	0.3695
1300.	128.917	246.174	116941.	-156.219	40.7239
1350.	129.343	251.047	123398.	-159.641	40.7496
1398.150	129.706	255.586	129635.	-162.868	40.7740
	cyclowollastonite (= "pseudowollastonite")				
1398.150	124.159	256.828	131371.	-162.868	40.9142
1400.	124.176	256.992	131600.	-162.992	40.9157
1450.	124.633	261.358	137821.	-166.309	40.9564
1500.	125.066	265.590	144063.	-169.548	40.9972
(2 sigma)	2.315	0.968	1032.	0.685	0.5886
1550.	125.478	269.698	150327.	-172.713	41.0381
1600.	125.869	273.688	156611.	-175.806	41.0791
1650.	126.241	277.567	162913.	-178.831	41.1201
1700.	126.597	281.341	169234.	-181.791	41.1612
1750.	126.936	285.015	175573.	-184.688	41.2023
(2 sigma)	2.652	1.220	1478.	0.699	0.8142
1800.	127.261	288.596	181928.	-187.525	41.2434
(2 sigma)	2.712	1.277	1589.	0.706	0.8601

Table 61. Thermochemical properties of stable phases with the composition $CaSiO_3$ at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
			wollastonite			
200.	-1633703.	-1577216.	411.926	-88836.	-89253.	23.310
250.	-1634371.	-1563007.	326.572	-88864.	-89354.	18.669
(2 sigma)	---	---	---	741.	657.	0.137
273.15	-1634543.	-1556391.	297.629	-88876.	-89399.	17.096
298.15	-1634651.	-1549232.	271.419	-88888.	-89446.	15.671
(2 sigma)	---	---	---	741.	644.	0.113
300.	-1634656.	-1548702.	269.653	-88889.	-89449.	15.574
350.	-1634672.	-1534372.	228.992	-88910.	-89541.	13.363
400.	-1634494.	-1520054.	198.499	-88933.	-89630.	11.700
450.	-1634178.	-1505767.	174.785	-88966.	-89715.	10.414
500.	-1633765.	-1491520.	155.818	-89016.	-89796.	9.381
(2 sigma)	---	---	---	741.	610.	0.064
550.	-1633286.	-1477319.	140.304	-89088.	-89870.	8.535
600.	-1632767.	-1463162.	127.380	-89187.	-89937.	7.830
650.	-1632228.	-1449050.	116.447	-89319.	-89995.	7.232
700.	-1631686.	-1434980.	107.079	-89486.	-90041.	6.719
750.	-1631991.	-1420912.	98.961	-89693.	-90073.	6.273
(2 sigma)	---	---	---	743.	611.	0.043
800.	-1631375.	-1406860.	91.858	-89943.	-90091.	5.882
850.	-1630826.	-1392845.	85.594	-90950.	-90086.	5.536
900.	-1630351.	-1378861.	80.027	-90870.	-90037.	5.226
950.	-1629954.	-1364900.	75.047	-90775.	-89994.	4.948
1000.	-1629639.	-1350958.	70.567	-90669.	-89955.	4.699
(2 sigma)	---	---	---	745.	657.	0.034
1050.	-1629410.	-1337030.	66.514	-90557.	-89922.	4.473
1100.	-1629269.	-1323111.	62.829	-90443.	-89895.	4.269
1150.	-1637092.	-1308916.	59.453	-90331.	-89872.	4.082
1200.	-1636194.	-1294667.	56.355	-90224.	-89855.	3.911
1250.	-1635289.	-1280455.	53.507	-90125.	-89842.	3.754
(2 sigma)	---	---	---	752.	742.	0.031
1300.	-1634378.	-1266280.	50.880	-90037.	-89832.	3.609
1350.	-1633463.	-1252139.	48.448	-89963.	-89826.	3.476
1398.150	-1632579.	-1238554.	46.272	-89906.	-89822.	3.356
			cyclowollastonite (= "pseudowollastonite")			
1398.150	-1630843.	-1238554.	46.272	-88171.	-89822.	3.356
1400.	-1630819.	-1238035.	46.192	-88179.	-89824.	3.351
1450.	-1630174.	-1224019.	44.094	-88413.	-89879.	3.238
1500.	-1629520.	-1210025.	42.137	-88662.	-89925.	3.131
(2 sigma)	---	---	---	1222.	855.	0.030
1550.	-1628859.	-1196052.	40.307	-88925.	-89963.	3.032
1600.	-1628190.	-1182101.	38.592	-89205.	-89992.	2.938
1650.	-1627514.	-1168172.	36.981	-89501.	-90012.	2.850
1700.	-1677339.	-1153812.	35.452	-89817.	-90023.	2.766
1750.	-1676504.	-1138427.	33.980	-90151.	-90024.	2.687
(2 sigma)	---	---	---	1650.	1020.	0.030
1800.	-1828491.	-1119141.	32.477	-90506.	-90015.	2.612
(2 sigma)	---	---	---	1757.	1062.	0.031

Table 62. Thermophysical values for wollastonite, $CaSiO_3$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	65.696	50.950	-7572.	-88.810	39.5612
250.	77.862	66.995	-3965.	-82.857	39.6874
(2 sigma)	0.075	0.689	3.	0.689	0.1482
273.15	82.290	74.088	-2111.	-81.815	39.7403
298.15	86.456	81.479	0.	-81.479	39.7940
(2 sigma)	0.076	0.689	0.	0.689	0.0986
300.	86.742	82.015	160.	-81.481	39.7978
350.	93.556	95.919	4675.	-82.563	39.8948
400.	98.972	108.778	9493.	-85.047	39.9804
450.	103.389	120.699	14555.	-88.354	40.0564
500.	107.062	131.788	19819.	-92.149	40.1243
(2 sigma)	0.118	0.688	17.	0.688	0.0807
550.	110.165	142.141	25252.	-96.229	40.1854
600.	112.818	151.844	30828.	-100.463	40.2406
650.	115.108	160.967	36528.	-104.770	40.2909
700.	117.102	169.572	42334.	-109.094	40.3370
750.	118.849	177.712	48234.	-113.400	40.3795
(2 sigma)	0.180	0.690	50.	0.688	0.0745
800.	120.387	185.432	54216.	-117.663	40.4191
850.	121.748	192.772	60270.	-121.867	40.4562
900.	122.955	199.766	66388.	-126.002	40.4911
950.	124.029	206.443	72563.	-130.061	40.5242
1000.	124.987	212.830	78789.	-134.041	40.5558
(2 sigma)	0.260	0.693	80.	0.688	0.1827
1050.	125.842	218.949	85060.	-137.940	40.5860
1100.	126.605	224.821	91371.	-141.756	40.6152
1150.	127.286	230.464	97719.	-145.491	40.6434
1200.	127.894	235.895	104099.	-149.146	40.6709
1250.	128.435	241.127	110507.	-152.721	40.6977
(2 sigma)	0.837	0.696	145.	0.688	0.3695
1300.	128.917	246.174	116941.	-156.219	40.7239
1350.	129.343	251.047	123398.	-159.641	40.7496
1398.150	129.706	255.586	129635.	-162.868	40.7740
1400.	129.719	255.758	129875.	-162.990	40.7750
1450.	130.048	260.316	136369.	-166.268	40.8000
1500.	130.335	264.730	142879.	-169.477	40.8247
(2 sigma)	1.868	0.753	438.	0.688	0.5803
1550.	130.583	269.007	149402.	-172.619	40.8491
1600.	130.794	273.157	155937.	-175.696	40.8734
1650.	130.972	277.184	162481.	-178.711	40.8974
1700.	131.117	281.096	169033.	-181.665	40.9214
1750.	131.233	284.899	175592.	-184.561	40.9452
(2 sigma)	3.333	0.970	1062.	0.692	0.8008
1800.	131.321	288.597	182156.	-187.399	40.9689
(2 sigma)	3.678	1.041	1235.	0.695	0.8456

Table 63. Thermochemical properties of wollastonite, $CaSiO_3$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-1633703.	-1577216.	411.926	-88836.	-89253.	23.310
250.	-1634371.	-1563007.	326.572	-88864.	-89354.	18.669
(2 sigma)	---	---	---	741.	657.	0.137
273.15	-1634543.	-1556391.	297.629	-88876.	-89399.	17.096
298.15	-1634651.	-1549232.	271.419	-88888.	-89446.	15.671
(2 sigma)	---	---	---	741.	644.	0.113
300.	-1634656.	-1548702.	269.653	-88889.	-89449.	15.574
350.	-1634672.	-1534372.	228.992	-88910.	-89541.	13.363
400.	-1634494.	-1520054.	198.499	-88933.	-89630.	11.704
450.	-1634178.	-1505767.	174.785	-88966.	-89715.	10.414
500.	-1633765.	-1491520.	155.818	-89016.	-89796.	9.381
(2 sigma)	---	---	---	741.	610.	0.064
550.	-1633286.	-1477319.	140.304	-89088.	-89870.	8.535
600.	-1632767.	-1463162.	127.380	-89187.	-89937.	7.830
650.	-1632228.	-1449050.	116.447	-89319.	-89995.	7.232
700.	-1631686.	-1434980.	107.079	-89486.	-90041.	6.719
750.	-1631991.	-1420912.	98.961	-89693.	-90073.	6.273
(2 sigma)	---	---	---	743.	611.	0.043
800.	-1631375.	-1406860.	91.858	-89943.	-90091.	5.882
850.	-1630826.	-1392845.	85.594	-90950.	-90086.	5.536
900.	-1630351.	-1378861.	80.027	-90870.	-90037.	5.226
950.	-1629954.	-1364900.	75.047	-90775.	-89994.	4.948
1000.	-1629639.	-1350958.	70.567	-90669.	-89955.	4.699
(2 sigma)	---	---	---	745.	657.	0.034
1050.	-1629410.	-1337030.	66.514	-90557.	-89922.	4.473
1100.	-1629269.	-1323111.	62.829	-90443.	-89895.	4.269
1150.	-1637092.	-1308916.	59.453	-90331.	-89872.	4.082
1200.	-1636194.	-1294667.	56.355	-90224.	-89855.	3.911
1250.	-1635289.	-1280455.	53.507	-90125.	-89842.	3.754
(2 sigma)	---	---	---	752.	742.	0.031
1300.	-1634378.	-1266280.	50.880	-90037.	-89832.	3.609
1350.	-1633463.	-1252139.	48.448	-89963.	-89826.	3.476
1398.150	-1632579.	-1238554.	46.272	-89906.	-89822.	3.356
1400.	-1632545.	-1238033.	46.192	-89905.	-89822.	3.351
1450.	-1631625.	-1223960.	44.092	-89865.	-89819.	3.236
1500.	-1630704.	-1209918.	42.133	-89846.	-89818.	3.128
(2 sigma)	---	---	---	850.	855.	0.030
1550.	-1629784.	-1195907.	40.302	-89850.	-89817.	3.027
1600.	-1628864.	-1181925.	38.586	-89879.	-89816.	2.932
1650.	-1627946.	-1167973.	36.975	-89934.	-89813.	2.843
1700.	-1677540.	-1153598.	35.446	-90018.	-89808.	2.759
1750.	-1676485.	-1138203.	33.973	-90132.	-89800.	2.680
(2 sigma)	---	---	---	1279.	996.	0.030
1800.	-1828263.	-1118915.	32.470	-90277.	-89789.	2.606
(2 sigma)	---	---	---	1423.	1029.	0.030

Table 64. Thermophysical values for cyclowollastonite (= "pseudo-wollastonite"), $CaSiO_3$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	69.327	55.409	-7897.	-94.893	40.1374
250.	81.283	72.268	-4108.	-88.700	40.1453
(2 sigma)	1.149	0.975	59.	0.899	0.1800
273.15	85.285	79.646	-2179.	-87.622	40.1508
298.15	88.906	87.276	0.	-87.276	40.1578
(2 sigma)	1.290	0.904	0.	0.904	0.1244
300.	89.150	87.826	165.	-87.277	40.1584
350.	94.798	102.015	4770.	-88.385	40.1758
400.	99.098	114.966	9622.	-90.910	40.1968
450.	102.511	126.842	14666.	-94.252	40.2210
500.	105.304	137.792	19863.	-98.066	40.2478
(2 sigma)	0.958	0.884	236.	0.867	0.0994
550.	107.646	147.941	25188.	-102.144	40.2769
600.	109.646	157.396	30622.	-106.359	40.3078
650.	111.380	166.242	36149.	-110.629	40.3403
700.	112.903	174.553	41756.	-114.901	40.3742
750.	114.255	182.390	47436.	-119.142	40.4092
(2 sigma)	0.884	0.872	389.	0.822	0.1000
800.	115.466	189.803	53180.	-123.328	40.4452
850.	116.559	196.836	58981.	-127.447	40.4820
900.	117.551	203.527	64834.	-131.490	40.5195
950.	118.459	209.907	70734.	-135.450	40.5576
1000.	119.292	216.005	76678.	-139.327	40.5962
(2 sigma)	1.406	0.798	519.	0.785	0.1913
1050.	120.061	221.844	82663.	-143.118	40.6352
1100.	120.774	227.446	88684.	-146.825	40.6746
1150.	121.438	232.830	94739.	-150.448	40.7142
1200.	122.057	238.011	100827.	-153.989	40.7542
1250.	122.636	243.006	106944.	-157.450	40.7943
(2 sigma)	1.905	0.812	794.	0.744	0.3748
1300.	123.180	247.826	113090.	-160.834	40.8346
1350.	123.693	252.485	119262.	-164.143	40.8751
1398.150	124.159	256.828	125229.	-167.260	40.9142
1400.	124.176	256.992	125459.	-167.379	40.9157
1450.	124.633	261.358	131679.	-170.545	40.9564
1500.	125.066	265.590	137921.	-173.643	40.9972
(2 sigma)	2.315	0.968	1236.	0.709	0.5886
1550.	125.478	269.698	144185.	-176.675	41.0381
1600.	125.869	273.688	150469.	-179.645	41.0791
1650.	126.241	277.567	156772.	-182.554	41.1201
1700.	126.597	281.341	163093.	-185.404	41.1612
1750.	126.936	285.015	169431.	-188.198	41.2023
(2 sigma)	2.652	1.220	1804.	0.691	0.8142
1800.	127.261	288.596	175786.	-190.937	41.2434
(2 sigma)	2.712	1.277	1930.	0.690	0.8601

Table 65. Thermochemical properties of cyclowollastonite (= "pseudo-wollastonite"), $CaSiO_3$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-1627886.	-1572291.	410.640	-83019.	-84328.	22.024
250.	-1628372.	-1558326.	325.594	-82865.	-84673.	17.691
(2 sigma)	---	---	---	1012.	896.	0.187
273.15	-1628470.	-1551835.	296.758	-82803.	-84843.	16.225
298.15	-1628510.	-1544819.	270.646	-82746.	-85032.	14.897
(2 sigma)	---	---	---	1021.	879.	0.154
300.	-1628510.	-1544300.	268.886	-82743.	-85047.	14.808
350.	-1628434.	-1530268.	228.380	-82672.	-85437.	12.751
400.	-1628223.	-1516258.	198.003	-82662.	-85834.	11.209
450.	-1627926.	-1502279.	174.380	-82714.	-86227.	10.009
500.	-1627579.	-1488337.	155.485	-82830.	-86612.	9.048
(2 sigma)	---	---	---	1073.	796.	0.083
550.	-1627208.	-1474430.	140.030	-83010.	-86982.	8.261
600.	-1626832.	-1460558.	127.153	-83252.	-87333.	7.603
650.	-1626466.	-1446717.	116.260	-83556.	-87661.	7.045
700.	-1626122.	-1432903.	106.924	-83922.	-87964.	6.564
750.	-1626647.	-1419076.	98.833	-84349.	-88238.	6.145
(2 sigma)	---	---	---	1072.	717.	0.050
800.	-1626269.	-1405251.	91.753	-84837.	-88482.	5.777
850.	-1625973.	-1391447.	85.508	-86097.	-88688.	5.450
900.	-1625763.	-1377658.	79.957	-86282.	-88835.	5.156
950.	-1625640.	-1363878.	74.991	-86462.	-88972.	4.892
1000.	-1625607.	-1350102.	70.522	-86638.	-89099.	4.654
(2 sigma)	---	---	---	1010.	704.	0.037
1050.	-1625665.	-1336326.	66.479	-86813.	-89218.	4.438
1100.	-1625815.	-1322545.	62.802	-86989.	-89328.	4.242
1150.	-1633930.	-1308474.	59.433	-87169.	-89431.	4.062
1200.	-1633325.	-1294337.	56.341	-87354.	-89525.	3.897
1250.	-1632711.	-1280225.	53.498	-87546.	-89612.	3.745
(2 sigma)	---	---	---	1014.	752.	0.031
1300.	-1632088.	-1266138.	50.874	-87747.	-89690.	3.604
1350.	-1631458.	-1252075.	48.446	-87957.	-89761.	3.473
1398.150	-1630843.	-1238554.	46.272	-88171.	-89822.	3.356
1400.	-1630819.	-1238035.	46.192	-88179.	-89824.	3.351
1450.	-1630174.	-1224019.	44.094	-88413.	-89879.	3.238
1500.	-1629520.	-1210025.	42.137	-88662.	-89925.	3.131
(2 sigma)	---	---	---	1222.	855.	0.030
1550.	-1628859.	-1196052.	40.307	-88925.	-89963.	3.032
1600.	-1628190.	-1182101.	38.592	-89205.	-89992.	2.938
1650.	-1627514.	-1168172.	36.981	-89501.	-90012.	2.850
1700.	-1677339.	-1153812.	35.452	-89817.	-90023.	2.766
1750.	-1676504.	-1138427.	33.980	-90151.	-90024.	2.687
(2 sigma)	---	---	---	1650.	1020.	0.030
1800.	-1828491.	-1119141.	32.477	-90506.	-90015.	2.612
(2 sigma)	---	---	---	1757.	1062.	0.031

Table 66. Thermophysical values for bicchulite, $Ca_2Al_2SiO_6(OH)_2$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	178.990	132.525	-21044.	-237.746	103.1788
250.	216.623	176.750	-11100.	-221.149	103.3668
(2 sigma)	---	19.874	---	19.874	1.5404
273.15	230.317	196.546	-5923.	-218.228	103.4538
298.15	243.200	217.285	0.	-217.285	103.5478
(2 sigma)	---	19.874	---	19.874	1.5335
300.	244.086	218.792	451.	-217.289	103.5548
350.	265.161	258.066	13203.	-220.343	103.7427
400.	281.913	294.607	26895.	-227.369	103.9307
450.	295.582	328.627	41344.	-236.752	104.1187
500.	306.959	360.376	56415.	-247.545	104.3066
(2 sigma)	---	19.874	---	19.874	1.6092
550.	316.578	390.096	72010.	-259.168	104.4946
600.	324.813	418.004	88050.	-271.253	104.6826
650.	331.936	444.290	104473.	-283.563	104.8705
700.	338.150	469.122	121229.	-295.938	105.0585
750.	343.608	492.642	138275.	-308.275	105.2465
(2 sigma)	---	19.874	---	19.874	1.9015
800.	348.430	514.975	155579.	-320.502	105.4344
850.	352.713	536.229	173109.	-332.571	105.6224
900.	356.531	556.500	190842.	-344.453	105.8104
950.	359.946	575.870	208756.	-356.127	105.9983
1000.	363.010	594.412	226831.	-367.581	106.1863
(2 sigma)	---	19.874	---	19.874	2.3348
1050.	365.765	612.191	245052.	-378.809	106.3743
1100.	368.246	629.265	263403.	-389.808	106.5622
1150.	370.484	645.684	281872.	-400.578	106.7502
1200.	372.504	661.495	300448.	-411.122	106.9381
1250.	374.329	676.739	319119.	-421.444	107.1261
(2 sigma)	---	19.874	---	19.874	2.8454

Table 67. Thermochemical properties of bicchulite, $Ca_2Al_2SiO_6(OH)_2$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-4332877.	-4158124.	1085.990	---	---	---
250.	-4335695.	-4114080.	859.589	---	---	---
(2 sigma)	---	---	---	---	---	---
273.15	-4336559.	-4093517.	782.805	-193805.	-188976.	36.138
298.15	-4337238.	-4071241.	713.264	-194835.	-188488.	33.022
(2 sigma)	---	---	---	18768.	12913.	2.262
300.	-4337279.	-4069590.	708.578	-194909.	-188449.	32.812
350.	-4337955.	-4024911.	600.685	-196836.	-187218.	27.941
400.	-4337956.	-3980184.	519.758	-238395.	-182818.	23.874
450.	-4337454.	-3935488.	456.819	-238041.	-175891.	20.417
500.	-4336582.	-3890869.	406.476	-237617.	-169007.	17.656
(2 sigma)	---	---	---	18768.	9002.	0.940
550.	-4335444.	-3846351.	365.296	-237141.	-162169.	15.402
600.	-4334125.	-3801945.	330.988	-236629.	-155376.	13.527
650.	-4332695.	-3757654.	301.969	-236095.	-148626.	11.944
700.	-4331215.	-3713476.	277.103	-235551.	-141918.	10.590
750.	-4331407.	-3669330.	255.555	-235007.	-135249.	9.420
(2 sigma)	---	---	---	18768.	4416.	0.308
800.	-4329755.	-3625246.	236.704	-234472.	-128616.	8.398
850.	-4328254.	-3581261.	220.077	-234667.	-122011.	7.498
900.	-4326933.	-3537359.	205.303	-233753.	-115410.	6.698
950.	-4347075.	-3492878.	192.052	-232806.	-108862.	5.986
1000.	-4345914.	-3447951.	180.102	-231834.	-102363.	5.347
(2 sigma)	---	---	---	18768.	2708.	0.141
1050.	-4344881.	-3403079.	169.294	-230847.	-95914.	4.771
1100.	-4343988.	-3358253.	159.470	-229852.	-89512.	4.251
1150.	-4358989.	-3312903.	150.477	-228857.	-83155.	3.777
1200.	-4356518.	-3267474.	142.229	-227867.	-76841.	3.345
1250.	-4354006.	-3222149.	134.646	-226890.	-70569.	2.949
(2 sigma)	---	---	---	18768.	6674.	0.279

Table 68. Thermophysical values for gehlenite, $Ca_2Al_2SiO_7$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	157.139	137.516	-17976.	-227.398	90.0044
250.	184.553	175.645	-9407.	-213.274	90.1287
(2 sigma)	0.533	1.024	27.	1.019	0.2395
273.15	195.180	192.461	-5010.	-210.802	90.1863
298.15	205.390	210.004	0.	-210.004	90.2485
(2 sigma)	0.601	1.019	0.	1.019	0.2312
300.	206.098	211.276	381.	-210.008	90.2531
350.	223.067	244.372	11126.	-212.582	90.3774
400.	236.587	275.074	22630.	-218.499	90.5017
450.	247.494	303.592	34742.	-226.388	90.6260
500.	256.399	330.144	47346.	-235.452	90.7503
(2 sigma)	1.099	1.100	169.	1.022	0.3329
550.	263.749	354.937	60356.	-245.200	90.8747
600.	269.877	378.157	73701.	-255.323	90.9990
650.	275.035	399.968	87327.	-265.619	91.1233
700.	279.418	420.515	101191.	-275.956	91.2476
750.	283.178	439.924	115259.	-286.246	91.3719
(2 sigma)	1.196	1.235	359.	1.047	0.5892
800.	286.438	458.307	129501.	-296.431	91.4963
850.	289.294	475.760	143896.	-306.471	91.6206
900.	291.826	492.368	158425.	-316.341	91.7449
950.	294.099	508.208	173074.	-326.025	91.8692
1000.	296.169	523.347	187831.	-335.516	91.9935
(2 sigma)	1.981	1.284	538.	1.075	0.8753
1050.	298.080	537.844	202688.	-344.808	92.1179
1100.	299.871	551.752	217637.	-353.900	92.2422
1150.	301.576	565.120	232674.	-362.795	92.3665
1200.	303.222	577.990	247794.	-371.495	92.4908
1250.	304.834	590.401	262995.	-380.004	92.6151
(2 sigma)	1.933	1.360	839.	1.096	1.1696
1300.	306.433	602.388	278277.	-388.328	92.7395
1350.	308.038	613.983	293639.	-396.472	92.8638
1400.	309.665	625.215	309081.	-404.442	92.9881
1450.	311.328	636.110	324606.	-412.244	93.1124
1500.	313.040	646.693	340215.	-419.883	93.2367
(2 sigma)	4.049	1.373	1006.	1.112	1.4672
1550.	314.812	656.987	355911.	-427.367	93.3611
1600.	316.654	667.010	371697.	-434.699	93.4854
1650.	318.575	676.783	387578.	-441.888	93.6097
1700.	320.584	686.323	403556.	-448.937	93.7340
1750.	322.687	695.647	419638.	-455.854	93.8583
(2 sigma)	10.352	1.659	1970.	1.125	1.7664
1800.	324.891	704.768	435827.	-462.642	93.9827
(2 sigma)	12.039	1.841	2434.	1.128	1.8263

Table 69. Thermochemical properties of gehlenite, $Ca_2Al_2SiO_7$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-3980020.	-3849503.	1005.386	-722656.	-735417.	192.071
250.	-3982126.	-3816609.	797.436	-720692.	-738836.	154.371
(2 sigma)	---	---	---	2537.	2422.	0.506
273.15	-3982778.	-3801252.	726.915	-719792.	-740557.	141.617
298.15	-3983286.	-3784613.	663.048	-718812.	-742501.	130.083
(2 sigma)	---	---	---	2538.	2403.	0.421
300.	-3983317.	-3783380.	658.745	-718739.	-742648.	129.306
350.	-3983810.	-3750010.	559.658	-716736.	-746790.	111.452
400.	-3983787.	-3716607.	485.339	-714681.	-751223.	98.100
450.	-3983397.	-3683230.	427.538	-712587.	-755916.	87.744
500.	-3982753.	-3649910.	381.303	-710470.	-760844.	79.485
(2 sigma)	---	---	---	2568.	2324.	0.243
550.	-3981950.	-3616664.	343.482	-708345.	-765984.	72.747
600.	-3981064.	-3583495.	311.971	-706225.	-771318.	67.149
650.	-3980156.	-3550401.	285.314	-704122.	-776828.	62.427
700.	-3979280.	-3517376.	262.470	-702044.	-782499.	58.391
750.	-3980151.	-3484338.	242.671	-699997.	-788317.	54.903
(2 sigma)	---	---	---	2627.	2236.	0.156
800.	-3979245.	-3451315.	225.348	-697989.	-794271.	51.861
850.	-3978552.	-3418342.	210.066	-131830.	-159923.	9.828
900.	-3978092.	-3385403.	196.484	-132136.	-161567.	9.377
950.	-3999141.	-3351835.	184.297	-132438.	-163194.	8.973
1000.	-3998926.	-3317773.	173.303	-132737.	-164805.	8.608
(2 sigma)	---	---	---	2671.	2174.	0.114
1050.	-3998870.	-3283717.	163.356	-133035.	-166401.	8.278
1100.	-3998977.	-3249660.	154.313	-133333.	-167982.	7.977
1150.	-4014993.	-3215034.	146.031	-133631.	-169551.	7.701
1200.	-4013546.	-3180284.	138.434	-133927.	-171106.	7.448
1250.	-4012058.	-3145595.	131.447	-134221.	-172649.	7.215
(2 sigma)	---	---	---	2730.	2152.	0.090
1300.	-4010527.	-3110967.	125.000	-134510.	-174181.	6.999
1350.	-4008949.	-3076398.	119.033	-134793.	-175701.	6.798
1400.	-4007323.	-3041889.	113.494	-135068.	-177211.	6.612
1450.	-4005644.	-3007439.	108.340	-135332.	-178711.	6.438
1500.	-4003907.	-2973047.	103.531	-135581.	-180203.	6.275
(2 sigma)	---	---	---	2753.	2182.	0.076
1550.	-4002108.	-2938715.	99.034	-135814.	-181686.	6.123
1600.	-4000240.	-2904441.	94.820	-136025.	-183163.	5.980
1650.	-3998298.	-2870227.	90.864	-136212.	-184633.	5.845
1700.	-4046784.	-2835624.	87.128	-136371.	-186098.	5.718
1750.	-4044531.	-2800034.	83.576	-136498.	-187558.	5.598
(2 sigma)	---	---	---	3209.	2259.	0.067
1800.	-4347847.	-2756663.	79.996	-136589.	-189016.	5.485
(2 sigma)	---	---	---	3511.	2281.	0.066

Table 70. Thermophysical values for prehnite, $Ca_2Al_2Si_3O_{10}(OH)_2$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	244.310	177.684	-28569.	-320.529	139.9306
250.	293.554	237.707	-15074.	-298.002	140.1868
(2 sigma)	0.346	0.755	16.	0.753	1.6079
273.15	312.686	264.555	-8053.	-294.035	140.3054
298.15	331.165	292.751	0.	-292.751	140.4334
(2 sigma)	0.414	0.753	0.	0.753	1.5934
300.	332.451	294.804	614.	-292.757	140.4429
350.	363.534	348.472	18041.	-296.925	140.6991
400.	388.759	398.718	36870.	-306.543	140.9553
450.	409.525	445.744	56843.	-319.426	141.2114
500.	426.825	489.814	77765.	-334.285	141.4676
(2 sigma)	2.111	0.975	259.	0.760	1.6296
550.	441.379	531.197	99480.	-350.324	141.7238
600.	453.721	570.146	121866.	-367.036	141.9799
650.	464.249	606.890	144822.	-384.086	142.2361
700.	473.272	641.633	168266.	-401.253	142.4923
750.	481.029	674.556	192128.	-418.386	142.7484
(2 sigma)	2.968	1.793	892.	0.874	1.8704
800.	487.712	705.820	216351.	-435.381	143.0046
850.	493.472	735.564	240884.	-452.172	143.2608
900.	498.434	763.915	265685.	-468.709	143.5170
950.	502.701	790.981	290716.	-484.964	143.7731
1000.	506.356	816.861	315945.	-500.917	144.0293
(2 sigma)	3.975	2.544	1627.	1.125	2.2614
1050.	509.472	841.644	341342.	-516.556	144.2855
1100.	512.109	865.407	366884.	-531.876	144.5416
1150.	514.316	888.222	392546.	-546.877	144.7978
1200.	516.140	910.151	418309.	-561.560	145.0540
1250.	517.616	931.251	444154.	-575.928	145.3101
(2 sigma)	6.144	3.246	2584.	1.419	2.7389

Table 71. Thermochemical properties of prehnite, $Ca_2Al_2Si_3O_{10}(OH)_2$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

T	Formation from the Elements			Formation from the Oxides		
K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-6190713.	-5942974.	1552.144	---	---	---
250.	-6194593.	-5880553.	1228.673	---	---	---
(2 sigma)	---	---	---	---	---	---
273.15	-6195829.	-5851415.	1118.969	-232004.	-225155.	43.057
298.15	-6196820.	-5819846.	1019.612	-233078.	-224480.	39.328
(2 sigma)	---	---	---	1882.	1827.	0.320
300.	-6196881.	-5817507.	1012.917	-233154.	-224427.	39.076
350.	-6197907.	-5754181.	858.764	-235126.	-222814.	33.253
400.	-6197949.	-5690779.	743.139	-276678.	-218029.	28.472
450.	-6197231.	-5627419.	653.213	-276282.	-210720.	24.460
500.	-6195931.	-5564171.	581.285	-275805.	-203461.	21.255
(2 sigma)	---	---	---	1945.	1796.	0.188
550.	-6194195.	-5501076.	522.448	-275291.	-196251.	18.638
600.	-6192143.	-5438154.	473.433	-274776.	-189088.	16.462
650.	-6189874.	-5375412.	431.973	-274293.	-181968.	14.623
700.	-6187473.	-5312851.	396.450	-273873.	-174882.	13.050
750.	-6186684.	-5250391.	365.669	-273541.	-167823.	11.688
(2 sigma)	---	---	---	2220.	1763.	0.123
800.	-6184010.	-5188059.	338.745	-273319.	-160783.	10.498
850.	-6181461.	-5125891.	314.999	-275365.	-153738.	9.448
900.	-6179080.	-5063868.	293.899	-274152.	-146618.	8.509
950.	-6198162.	-5001325.	274.992	-272907.	-139566.	7.674
1000.	-6195951.	-4938391.	257.955	-271652.	-132581.	6.925
(2 sigma)	---	---	---	2675.	1843.	0.096
1050.	-6193889.	-4875565.	242.546	-270408.	-125658.	6.251
1100.	-6191993.	-4812833.	228.542	-269194.	-118794.	5.641
1150.	-6206026.	-4749622.	215.734	-268026.	-111984.	5.086
1200.	-6202629.	-4686373.	203.992	-266920.	-105223.	4.580
1250.	-6199237.	-4623265.	193.196	-265891.	-98507.	4.116
(2 sigma)	---	---	---	3369.	2159.	0.090

Table 72. Thermopnysical values for zoisite, $Ca_2Al_3Si_3O_{12}(OH)$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	253.187	175.254	-29971.	-325.110	136.2311
250.	308.188	237.915	-15879.	-301.433	136.4800
(2 sigma)	0.367	0.760	17.	0.757	1.0162
273.15	329.389	266.151	-8495.	-297.251	136.5953
298.15	349.800	295.896	0.	-295.896	136.7198
(2 sigma)	0.439	0.757	0.	0.757	0.9945
300.	351.219	298.064	648.	-295.902	136.7290
350.	385.421	354.870	19096.	-300.310	136.9779
400.	413.084	408.204	39082.	-310.499	137.2268
450.	435.800	458.212	60322.	-324.163	137.4757
500.	454.690	505.136	82598.	-339.939	137.7246
(2 sigma)	2.227	0.989	275.	0.762	1.0239
550.	470.559	549.238	105741.	-356.982	137.9736
600.	483.996	590.774	129614.	-374.751	138.2225
650.	495.447	629.978	154107.	-392.890	138.4714
700.	505.249	667.063	179131.	-411.161	138.7203
750.	513.668	702.216	204609.	-429.404	138.9692
(2 sigma)	3.189	1.846	936.	0.878	1.2899
800.	520.912	735.604	230478.	-447.506	139.2182
850.	527.149	767.376	256684.	-465.395	139.4671
900.	532.515	797.663	283179.	-483.020	139.7160
950.	537.123	826.581	309923.	-500.347	139.9649
1000.	541.065	854.235	336880.	-517.355	140.2138
(2 sigma)	4.767	2.657	1743.	1.139	1.6967
1050.	544.419	880.717	364019.	-534.032	140.4628
1100.	547.251	906.111	391313.	-550.372	140.7117
1150.	549.616	930.491	418737.	-566.372	140.9606
1200.	551.562	953.925	446268.	-582.035	141.2095
1250.	553.131	976.474	473886.	-597.364	141.4584
(2 sigma)	7.762	3.538	2956.	1.455	2.1664

Table 73. Thermochemical properties of zoisite, $Ca_2Al_3Si_3O_{12}(OH)$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-6887201.	-6627758.	1730.992	---	---	---
250.	-6891657.	-6562340.	1371.125	---	---	---
(--- ma)	---	---	---	---	---	---
273.15	-6893086.	-6531778.	1249.075	-234896.	-231083.	44.190
298.15	-6894244.	-6498655.	1138.537	-235536.	-230706.	40.419
(2 sigma)	---	---	---	2250.	2193.	0.384
300.	-6894316.	-6496200.	1131.088	-235582.	-230676.	40.164
350.	-6895573.	-6429731.	959.584	-236758.	-229763.	34.290
400.	-6895747.	-6363159.	830.943	-257693.	-227240.	29.674
450.	-6895090.	-6296617.	730.892	-257630.	-223436.	25.936
500.	-6893801.	-6230185.	650.862	-257513.	-219643.	22.946
(2 sigma)	---	---	---	2343.	2152.	0.225
550.	-6892043.	-6163905.	585.398	-257375.	-215863.	20.501
600.	-6889947.	-6097801.	530.860	-257249.	-212094.	18.464
650.	-6887626.	-6031881.	484.728	-257161.	-208336.	16.742
700.	-6885173.	-5966146.	445.199	-257139.	-204581.	15.266
750.	-6884341.	-5900516.	410.948	-257204.	-200825.	13.987
(2 sigma)	---	---	---	2677.	2067.	0.144
800.	-6881641.	-5835016.	380.987	-257377.	-197062.	12.867
850.	-6879089.	-5769681.	354.561	-259813.	-193268.	11.877
900.	-6876737.	-5704491.	331.080	-258986.	-189377.	10.991
950.	-6906513.	-5638454.	310.024	-258121.	-185533.	10.201
1000.	-6904273.	-5571772.	291.039	-257240.	-181736.	9.493
(2 sigma)	---	---	---	3187.	2046.	0.107
1050.	-6902171.	-5505200.	273.869	-256364.	-177982.	8.854
1100.	-6900226.	-5438724.	258.263	-255511.	-174270.	8.275
1150.	-6914201.	-5371771.	243.993	-254699.	-170595.	7.749
1200.	-6910739.	-5304783.	230.911	-253943.	-166955.	7.267
1250.	-6907277.	-5237940.	218.881	-253259.	-163345.	6.826
(2 sigma)	---	---	---	4036.	2253.	0.094

Table 74. Thermophysical values for stable phases with the composition Ca_2SiO_4 at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
		Ca-olivine			
200.	97.496	75.402	-11176.	-131.282	58.9137
250.	115.197	99.254	-5815.	-122.515	59.0137
(2 sigma)	0.307	2.153	17.	2.152	0.9342
273.15	120.737	109.706	-3082.	-120.989	59.0600
298.15	125.690	120.499	0.	-120.499	59.1100
(2 sigma)	0.407	2.152	0.	2.152	0.9260
300.	126.025	121.278	233.	-120.502	59.1137
350.	133.898	141.321	6739.	-122.067	59.2137
400.	140.297	159.630	13598.	-125.634	59.3137
450.	145.851	176.482	20755.	-130.360	59.4137
500.	150.846	192.112	28174.	-135.763	59.5137
(2 sigma)	0.526	2.162	82.	2.153	1.0616
550.	155.417	206.706	35833.	-141.556	59.6137
600.	159.629	220.413	43710.	-147.562	59.7137
650.	163.510	233.345	51790.	-153.668	59.8137
700.	167.074	245.595	60056.	-159.801	59.9137
750.	170.322	257.234	68492.	-165.912	60.0137
(2 sigma)	0.433	2.182	185.	2.156	1.4860
800.	173.251	268.322	77083.	-171.968	60.1137
850.	175.859	278.905	85812.	-177.950	60.2137
900.	178.138	289.023	94663.	-183.842	60.3137
950.	180.084	298.708	103620.	-189.634	60.4137
970.	180.767	302.467	107229.	-191.922	60.4537
1000.	181.690	307.987	112666.	-195.322	60.5137
(2 sigma)	1.428	2.172	158.	2.159	2.0289
1050.	182.952	316.884	121783.	-200.900	60.6137
1100.	183.864	325.417	130955.	-206.367	60.7137
1120.	184.130	328.733	134635.	-208.523	60.7537
		bredigite			
1120.	185.297	341.377	148797.	-208.523	53.5615
1150.	186.587	346.292	154375.	-212.053	53.6185
1200.	188.814	354.280	163759.	-217.813	53.7135
1250.	191.135	362.034	173258.	-223.428	53.8085
(2 sigma)	2.241	1.488	2941.	1.941	2.8942
1300.	193.551	369.577	182875.	-228.905	53.9035
1350.	196.062	376.929	192614.	-234.251	53.9985
1400.	198.668	384.106	202482.	-239.476	54.0935
1450.	201.368	391.124	212483.	-244.584	54.1885
1500.	204.163	397.998	222621.	-249.584	54.2835
(2 sigma)	6.096	1.486	2960.	1.655	3.4552
1550.	207.053	404.739	232901.	-254.481	54.3785
1600.	210.037	411.360	243328.	-259.280	54.4735
1650.	213.117	417.870	253906.	-263.987	54.5685
1700.	216.291	424.279	264641.	-268.608	54.6635
1710.	216.937	425.549	266807.	-269.522	54.6825
		alpha-Ca_2SiO_4			
1710.	199.600	433.962	281193.	-269.522	54.9805
1750.	199.600	438.577	289177.	-273.333	55.0565
(2 sigma)	35.790	1.506	3100.	1.474	3.7697
1800.	199.600	444.200	299157.	-278.002	55.1515
(2 sigma)	35.790	1.735	3471.	1.446	3.8972

Table 75. Thermochemical properties of stable phases with the composition Ca_2SiO_4 at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
			Ca-olivine			
200.	-2316298.	-2239033.	584.775	-136444.	-137183.	35.828
250.	-2317181.	-2219600.	463.760	-136541.	-137356.	28.699
(2 sigma)	---	---	---	2563.	2065.	0.432
273.15	-2317393.	-2210554.	422.725	-136595.	-137429.	26.281
298.15	-2317527.	-2200769.	385.565	-136670.	-137502.	24.090
(2 sigma)	---	---	---	2563.	1972.	0.345
300.	-2317534.	-2200044.	383.062	-136676.	-137508.	23.942
350.	-2317574.	-2180456.	325.415	-136880.	-137631.	20.540
400.	-2317406.	-2160877.	282.181	-137140.	-137721.	17.984
450.	-2317089.	-2141329.	248.559	-137433.	-137776.	15.993
500.	-2316660.	-2121822.	221.665	-137743.	-137798.	14.396
(2 sigma)	---	---	---	2570.	1592.	0.166
550.	-2316149.	-2102363.	199.666	-138053.	-137788.	13.086
600.	-2315580.	-2082952.	181.337	-138355.	-137751.	11.992
650.	-2314974.	-2063591.	165.832	-138645.	-137688.	11.065
700.	-2314353.	-2044277.	152.546	-138921.	-137604.	10.268
750.	-2315409.	-2024934.	141.029	-139184.	-137501.	9.576
(2 sigma)	---	---	---	2583.	1169.	0.081
800.	-2314600.	-2005597.	130.952	-139440.	-137380.	8.970
850.	-2313904.	-1986306.	122.063	-140408.	-137239.	8.434
900.	-2313335.	-1967052.	114.165	-140248.	-137057.	7.955
950.	-2312905.	-1947827.	107.099	-140040.	-136885.	7.526
970.	-2312776.	-1940142.	104.477	-139947.	-136819.	7.368
1000.	-2312629.	-1928620.	100.741	-139800.	-136725.	7.142
(2 sigma)	---	---	---	2576.	888.	0.046
1050.	-2312522.	-1909423.	94.989	-139540.	-136577.	6.794
1100.	-2312599.	-1890227.	89.759	-139278.	-136442.	6.479
1120.	-2329460.	-1882425.	87.793	-139177.	-136392.	6.361
			bredigite			
1120.	-2315299.	-1882425.	87.793	-125015.	-136392.	6.361
1150.	-2314408.	-1870842.	84.976	-124819.	-136699.	6.209
1200.	-2312857.	-1851589.	80.598	-124444.	-137223.	5.973
1250.	-2311218.	-1832403.	76.572	-124005.	-137765.	5.757
(2 sigma)	---	---	---	1590.	933.	0.039
1300.	-2309485.	-1813284.	72.859	-123494.	-138325.	5.558
1350.	-2307651.	-1794234.	69.423	-122909.	-138906.	5.375
1400.	-2305710.	-1775254.	66.235	-122242.	-139511.	5.205
1450.	-2303656.	-1756345.	63.270	-121490.	-140140.	5.048
1500.	-2301482.	-1737509.	60.505	-120648.	-140798.	4.903
(2 sigma)	---	---	---	1633.	1168.	0.041
1550.	-2299182.	-1718747.	57.921	-119711.	-141484.	4.768
1600.	-2296750.	-1700062.	55.501	-118674.	-142203.	4.642
1650.	-2294180.	-1681455.	53.230	-117534.	-142956.	4.526
1700.	-2341975.	-1662478.	51.082	-116285.	-143744.	4.417
1710.	-2341386.	-1658483.	50.661	-116022.	-143907.	4.396
			alpha-Ca_2SiO_4			
1710.	-2327000.	-1658483.	50.661	-101635.	-143907.	4.396
1750.	-2325327.	-1642864.	49.037	-101283.	-144900.	4.325
(2 sigma)	---	---	---	1877.	1440.	0.043
1800.	-2628909.	-1615547.	46.882	-100885.	-146152.	4.241
(2 sigma)	---	---	---	2441.	1495.	0.043

Table 76. Thermophysical values for alpha-Ca_2SiO_4 at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5. Reference phase at 298.15 K is Ca olivine.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
1500.	199.600	407.809	239277.	-248.291	54.5815
(2 sigma)	35.790	5.848	9670.	1.725	3.1339
1550.	199.600	414.354	249257.	-253.543	54.6765
1600.	199.600	420.691	259237.	-258.668	54.7715
1650.	199.600	426.833	269217.	-263.671	54.8665
1700.	199.600	432.792	279197.	-268.558	54.9615
1710.	199.600	433.962	281193.	-269.522	54.9805
1750.	199.600	438.577	289177.	-273.333	55.0565
(2 sigma)	35.790	1.506	3100.	1.474	3.7697
1800.	199.600	444.200	299157.	-278.002	55.1515
(2 sigma)	35.790	1.735	3471.	1.446	3.8972

Table 77. Thermochemical properties of alpha-Ca_2SiO_4 at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

T	Formation from the Elements			Formation from the Oxides		
K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
1500.	-2284826.	-1735569.	60.438	-103992.	-138858.	4.835
(2 sigma)	---	---	---	9350.	1378.	0.048
1550.	-2282826.	-1717294.	57.872	-103355.	-140031.	4.719
1600.	-2280840.	-1699082.	55.469	-102765.	-141223.	4.610
1650.	-2278869.	-1680933.	53.214	-102223.	-142434.	4.509
1700.	-2327418.	-1662393.	51.079	-101729.	-143660.	4.414
1710.	-2327000.	-1658483.	50.661	-101635.	-143907.	4.396
1750.	-2325327.	-1642864.	49.037	-101283.	-144900.	4.325
(2 sigma)	---	---	---	1877.	1440.	0.043
1800.	-2628909.	-1615547.	46.882	-100885.	-146152.	4.241
(2 sigma)	---	---	---	2441.	1495.	0.043

Table 78. Thermophysical values for bredigite, Ca_2SiO_4, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	162.284	51.598	-15971.	-131.452	51.8135
250.	162.711	87.855	-7846.	-119.240	51.9085
(2 sigma)	14.480	16.855	692.	14.102	1.5483
273.15	162.940	102.275	-4077.	-117.200	51.9525
298.15	163.211	116.556	0.	-116.556	52.0000
(2 sigma)	14.242	14.336	0.	14.336	1.5433
300.	163.232	117.565	302.	-116.559	52.0035
350.	163.848	142.773	8479.	-118.548	52.0985
400.	164.558	164.697	16688.	-122.976	52.1935
450.	165.364	184.125	24936.	-128.711	52.2885
500.	166.264	201.593	33226.	-135.141	52.3835
(2 sigma)	12.786	7.359	2740.	12.776	1.6283
550.	167.259	217.486	41564.	-141.915	52.4785
600.	168.348	232.085	49954.	-148.829	52.5735
650.	169.533	245.606	58400.	-155.760	52.6685
700.	170.812	258.216	66909.	-162.633	52.7635
750.	172.186	270.047	75483.	-169.403	52.8585
(2 sigma)	9.979	2.893	5608.	10.105	1.9320
800.	173.654	281.206	84129.	-176.046	52.9535
850.	175.218	291.781	92850.	-182.545	53.0485
900.	176.876	301.842	101652.	-188.896	53.1435
950.	178.628	311.452	110539.	-195.095	53.2385
970.	179.356	315.181	114119.	-197.533	53.2765
1000.	180.476	320.661	119516.	-201.145	53.3335
(2 sigma)	6.132	1.363	7633.	7.929	2.3751
1050.	182.418	329.513	128588.	-207.048	53.4285
1100.	184.455	338.046	137760.	-212.810	53.5235
1120.	185.297	341.377	141457.	-215.076	53.5615
1150.	186.587	346.292	147036.	-218.435	53.6185
1200.	188.814	354.280	156420.	-223.929	53.7135
1250.	191.135	362.034	165918.	-229.299	53.8085
(2 sigma)	2.241	1.488	8547.	6.327	2.8942
1300.	193.551	369.577	175535.	-234.550	53.9035
1350.	196.062	376.929	185275.	-239.688	53.9985
1400.	198.668	384.106	195143.	-244.718	54.0935
1450.	201.368	391.124	205144.	-249.646	54.1885
1500.	204.163	397.998	215281.	-254.477	54.2835
(2 sigma)	6.096	1.486	8109.	5.231	3.4552
1550.	207.053	404.739	225561.	-259.216	54.3785
1600.	210.037	411.360	235988.	-263.867	54.4735
1650.	213.117	417.870	246567.	-268.435	54.5685
1700.	216.291	424.279	257301.	-272.925	54.6635
1710.	216.937	425.549	259468.	-273.814	54.6825
1750.	219.559	430.595	268197.	-277.340	54.7585
(2 sigma)	13.312	2.059	6203.	4.574	4.0408
1800.	222.923	436.828	279259.	-281.684	54.8535
(2 sigma)	14.917	2.342	5674.	4.490	4.1599

Table 79. Thermochemical properties of bredigite, Ca_2SiO_4, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-2313753.	-2231728.	582.867	-133899.	-129877.	33.920
250.	-2311873.	-2211442.	462.055	-131232.	-129198.	26.994
(2 sigma)	---	---	---	8611.	4447.	0.929
273.15	-2311048.	-2202180.	421.124	-130251.	-129055.	24.679
298.15	-2310188.	-2192254.	384.074	-129331.	-128987.	22.598
(2 sigma)	---	---	---	7931.	3718.	0.651
300.	-2310125.	-2191522.	381.578	-129268.	-128985.	22.458
350.	-2308495.	-2171886.	324.136	-127802.	-129060.	19.261
400.	-2306977.	-2152475.	281.084	-126711.	-129318.	16.887
450.	-2305569.	-2133248.	247.621	-125913.	-129695.	15.055
500.	-2304269.	-2114172.	220.866	-125351.	-130147.	13.596
(2 sigma)	---	---	---	5266.	1729.	0.181
550.	-2303078.	-2095221.	198.987	-124982.	-130646.	12.408
600.	-2301997.	-2076373.	180.764	-124773.	-131171.	11.419
650.	-2301024.	-2057611.	165.352	-124695.	-131708.	10.584
700.	-2300161.	-2038920.	152.146	-124729.	-132247.	9.868
750.	-2301078.	-2020214.	140.700	-124854.	-132781.	9.248
(2 sigma)	---	---	---	2631.	854.	0.059
800.	-2300215.	-2001519.	130.686	-125055.	-133303.	8.704
850.	-2299527.	-1982872.	121.852	-126030.	-133805.	8.223
900.	-2299007.	-1964261.	114.003	-125920.	-134266.	7.793
950.	-2298647.	-1945675.	106.981	-125782.	-134733.	7.408
970.	-2298546.	-1938245.	104.375	-125718.	-134922.	7.266
1000.	-2298439.	-1927104.	100.661	-125610.	-135208.	7.063
(2 sigma)	---	---	---	1428.	800.	0.042
1050.	-2298378.	-1908539.	94.945	-125396.	-135693.	6.750
1100.	-2298455.	-1889974.	89.747	-125134.	-136190.	6.467
1120.	-2315299.	-1882425.	87.793	-125015.	-136392.	6.361
1150.	-2314408.	-1870842.	84.976	-124819.	-136699.	6.209
1200.	-2312857.	-1851589.	80.598	-124444.	-137223.	5.973
1250.	-2311218.	-1832403.	76.572	-124005.	-137765.	5.757
(2 sigma)	---	---	---	1590.	933.	0.039
1300.	-2309485.	-1813284.	72.859	-123494.	-138325.	5.558
1350.	-2307651.	-1794234.	69.423	-122909.	-138906.	5.375
1400.	-2305710.	-1775254.	66.235	-122242.	-139511.	5.205
1450.	-2303656.	-1756345.	63.270	-121490.	-140140.	5.048
1500.	-2301482.	-1737509.	60.505	-120648.	-140798.	4.903
(2 sigma)	---	---	---	1633.	1168.	0.041
1550.	-2299182.	-1718747.	57.921	-119711.	-141484.	4.768
1600.	-2296750.	-1700062.	55.501	-118674.	-142203.	4.642
1650.	-2294180.	-1681455.	53.230	-117534.	-142956.	4.526
1700.	-2341975.	-1662478.	51.082	-116285.	-143744.	4.417
1710.	-2341386.	-1658483.	50.661	-116022.	-143907.	4.396
1750.	-2338968.	-1642536.	49.027	-114923.	-144572.	4.315
(2 sigma)	---	---	---	2989.	1444.	0.043
1800.	-2641468.	-1614835.	46.861	-113444.	-145439.	4.221
(2 sigma)	---	---	---	3588.	1507.	0.044

Table 80. Thermophysical values for Ca-olivine, Ca_2SiO_4, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C°_p J/(mol K)	S° J/(mol K)	$H^\circ_T - H^\circ_{298}$ J/mol	$[G^\circ_T - H^\circ_{298}]/T$ J/(mol K)	V° cm^3/mol
200.	97.496	75.402	-11176.	-131.282	58.9137
250.	115.197	99.254	-5815.	-122.515	59.0137
(2 sigma)	0.307	2.153	17.	2.152	0.9342
273.15	120.737	109.706	-3082.	-120.989	59.0600
298.15	125.690	120.499	0.	-120.499	59.1100
(2 sigma)	0.407	2.152	0.	2.152	0.9260
300.	126.025	121.278	233.	-120.502	59.1137
350.	133.898	141.321	6739.	-122.067	59.2137
400.	140.297	159.630	13598.	-125.634	59.3137
450.	145.851	176.482	20755.	-130.360	59.4137
500.	150.846	192.112	28174.	-135.763	59.5137
(2 sigma)	0.526	2.162	82.	2.153	1.0616
550.	155.417	206.706	35833.	-141.556	59.6137
600.	159.629	220.413	43710.	-147.562	59.7137
650.	163.510	233.345	51790.	-153.668	59.8137
700.	167.074	245.595	60056.	-159.801	59.9137
750.	170.322	257.234	68492.	-165.912	60.0137
(2 sigma)	0.433	2.182	185.	2.156	1.4860
800.	173.251	268.322	77083.	-171.968	60.1137
850.	175.859	278.905	85812.	-177.950	60.2137
900.	178.138	289.023	94663.	-183.842	60.3137
950.	180.084	298.708	103620.	-189.634	60.4137
970.	180.767	302.467	107229.	-191.922	60.4537
1000.	181.690	307.987	112666.	-195.322	60.5137
(2 sigma)	1.428	2.172	158.	2.159	2.0289
1050.	182.952	316.884	121783.	-200.900	60.6137
1100.	183.864	325.417	130955.	-206.367	60.7137
1120.	184.130	328.733	134635.	-208.523	60.7537
1150.	184.422	333.604	140164.	-211.723	60.8137
1200.	184.622	341.459	149391.	-216.966	60.9137
(2 sigma)	4.401	2.214	680.	2.159	2.6176

Table 81. Thermochemical properties of Ca-olivine, Ca_2SiO_4, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-2316298.	-2239033.	584.775	-136444.	-137183.	35.828
250.	-2317181.	-2219600.	463.760	-136541.	-137356.	28.699
(2 sigma)	---	---	---	2563.	2065.	0.432
273.15	-2317393.	-2210554.	422.725	-136595.	-137429.	26.281
298.15	-2317527.	-2200769.	385.565	-136670.	-137502.	24.090
(2 sigma)	---	---	---	2563.	1972.	0.345
300.	-2317534.	-2200044.	383.062	-136676.	-137508.	23.942
350.	-2317574.	-2180456.	325.415	-136880.	-137631.	20.540
400.	-2317406.	-2160877.	282.181	-137140.	-137721.	17.984
450.	-2317089.	-2141329.	248.559	-137433.	-137776.	15.993
500.	-2316660.	-2121822.	221.665	-137743.	-137798.	14.396
(2 sigma)	---	---	---	2570.	1592.	0.166
550.	-2316149.	-2102363.	199.666	-138053.	-137788.	13.086
600.	-2315580.	-2082952.	181.337	-138355.	-137751.	11.992
650.	-2314974.	-2063591.	165.832	-138645.	-137688.	11.065
700.	-2314353.	-2044277.	152.546	-138921.	-137604.	10.268
750.	-2315409.	-2024934.	141.029	-139184.	-137501.	9.576
(2 sigma)	---	---	---	2583.	1169.	0.081
800.	-2314600.	-2005597.	130.952	-139440.	-137380.	8.970
850.	-2313904.	-1986306.	122.063	-140408.	-137239.	8.434
900.	-2313335.	-1967052.	114.165	-140248.	-137057.	7.955
950.	-2312905.	-1947827.	107.099	-140040.	-136885.	7.526
970.	-2312776.	-1940142.	104.477	-139947.	-136819.	7.368
1000.	-2312629.	-1928620.	100.741	-139800.	-136725.	7.142
(2 sigma)	---	---	---	2576.	888.	0.046
1050.	-2312522.	-1909423.	94.989	-139540.	-136577.	6.794
1100.	-2312599.	-1890227.	89.759	-139278.	-136442.	6.479
1120.	-2329460.	-1882425.	87.793	-139177.	-136392.	6.361
1150.	-2328619.	-1870462.	84.959	-139030.	-136319.	6.192
1200.	-2327225.	-1850572.	80.553	-138812.	-136206.	5.929
(2 sigma)	---	---	---	2627.	895.	0.037

Table 82. Thermophysical values for larnite, Ca_2SiO_4, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T	C_p°	S°	$H_T^\circ - H_{298}^\circ$	$[G_T^\circ - H_{298}^\circ]/T$	V°
K	J/(mol K)	J/(mol K)	J/mol	J/(mol K)	cm^3/mol
200.	101.598	81.036	-11418.	-138.127	51.5499
250.	117.236	105.484	-5926.	-129.186	51.5742
(2 sigma)	0.269	1.289	12.	1.286	1.3890
273.15	122.974	116.122	-3144.	-127.632	51.5863
298.15	128.404	127.131	0.	-127.131	51.6000
(2 sigma)	0.250	1.286	0.	1.286	1.3890
300.	128.779	127.927	238.	-127.134	51.6010
350.	137.750	148.479	6910.	-128.736	51.6301
400.	144.982	167.361	13984.	-132.401	51.6610
450.	150.972	184.793	21387.	-137.266	51.6934
500.	156.039	200.969	29066.	-142.837	51.7272
(2 sigma)	0.488	1.281	72.	1.283	1.3893
550.	160.399	216.051	36980.	-148.815	51.7621
600.	164.202	230.174	45097.	-155.013	51.7980
650.	167.557	243.452	53392.	-161.310	51.8346
700.	170.545	255.981	61846.	-167.629	51.8720
750.	173.230	267.841	70442.	-173.918	51.9099
(2 sigma)	0.700	1.311	220.	1.279	1.3894
800.	175.659	279.099	79165.	-180.143	51.9483
850.	177.870	289.816	88004.	-186.282	51.9871
900.	179.895	300.041	96949.	-192.320	52.0262
950.	181.757	309.818	105991.	-198.249	52.0657
970.	182.461	313.612	109633.	-200.588	52.0815
1000.	183.478	319.185	115122.	-204.063	52.1054
(2 sigma)	0.832	1.374	410.	1.283	1.3895
1050.	185.074	328.176	124337.	-209.760	52.1453
1100.	186.561	336.821	133628.	-215.341	52.1854
1150.	187.949	345.144	142991.	-220.805	52.2256
1200.	189.249	353.171	152421.	-226.154	52.2660
1250.	190.471	360.922	161915.	-231.390	52.3065
(2 sigma)	0.923	1.456	628.	1.294	1.3904

Table 83. Thermochemical properties of larnite, Ca_2SiO_4, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-2306237.	-2230099.	582.442	-126383.	-128248.	33.495
250.	-2306988.	-2210965.	461.955	-126348.	-128721.	26.895
(2 sigma)	---	---	---	1348.	1105.	0.231
273.15	-2307151.	-2202065.	421.102	-126353.	-128940.	24.657
298.15	-2307224.	-2192443.	384.107	-126367.	-129176.	22.631
(2 sigma)	---	---	---	1348.	1064.	0.186
300.	-2307225.	-2191731.	381.614	-126368.	-129194.	22.495
350.	-2307100.	-2172487.	324.226	-126406.	-129662.	19.351
400.	-2306717.	-2153281.	281.189	-126451.	-130124.	16.992
450.	-2306153.	-2134133.	247.724	-126498.	-130580.	15.157
500.	-2305465.	-2115056.	220.958	-126548.	-131031.	13.689
(2 sigma)	---	---	---	1353.	911.	0.095
550.	-2304699.	-2096052.	199.066	-126603.	-131477.	12.487
600.	-2303890.	-2077119.	180.829	-126666.	-131918.	11.484
650.	-2303068.	-2058255.	165.403	-126739.	-132352.	10.636
700.	-2302259.	-2039454.	152.186	-126827.	-132781.	9.908
750.	-2303155.	-2020636.	140.730	-126931.	-133203.	9.277
(2 sigma)	---	---	---	1376.	795.	0.055
800.	-2302214.	-2001833.	130.706	-127055.	-133617.	8.724
850.	-2301409.	-1983084.	121.865	-127912.	-134017.	8.236
900.	-2300746.	-1964379.	114.010	-127659.	-134384.	7.799
950.	-2300231.	-1945707.	106.982	-127366.	-134765.	7.410
970.	-2300068.	-1938245.	104.375	-127239.	-134922.	7.266
1000.	-2299870.	-1927058.	100.659	-127040.	-135163.	7.060
(2 sigma)	---	---	---	1428.	800.	0.042
1050.	-2299666.	-1908423.	94.939	-126684.	-135578.	6.745
1100.	-2299623.	-1889794.	89.739	-126302.	-136010.	6.459
1150.	-2315488.	-1870603.	84.965	-125900.	-136460.	6.198
1200.	-2313892.	-1851294.	80.585	-125479.	-136928.	5.960
1250.	-2312258.	-1832052.	76.557	-125044.	-137414.	5.742
(2 sigma)	---	---	---	1515.	943.	0.039

Table 84. Thermophysical values for grossular, $Ca_3Al_2Si_3O_{12}$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	235.117	142.930	-28191.	-283.887	124.9446
250.	290.295	201.622	-14989.	-261.577	125.0676
(2 sigma)	0.191	3.744	9.	3.743	0.0727
273.15	310.963	228.252	-8024.	-257.628	125.1270
298.15	330.541	256.348	0.	-256.348	125.1926
(2 sigma)	0.160	3.743	0.	3.743	0.0462
300.	331.890	258.397	613.	-256.355	125.1975
350.	363.910	312.066	18041.	-260.520	125.3333
400.	389.041	362.365	36889.	-270.142	125.4740
450.	409.085	409.388	56861.	-283.030	125.6189
500.	425.281	453.357	77734.	-297.889	125.7673
(2 sigma)	0.168	3.745	26.	3.743	0.0589
550.	438.509	494.532	99340.	-313.914	125.9187
600.	449.408	533.169	121546.	-330.592	126.0727
650.	458.454	569.509	144250.	-347.587	126.2288
700.	466.010	603.769	167367.	-364.674	126.3867
750.	472.357	636.143	190830.	-381.703	126.5462
(2 sigma)	0.762	3.733	96.	3.742	0.0524
800.	477.718	666.804	214586.	-398.572	126.7070
850.	482.270	695.906	238589.	-415.213	126.8688
900.	486.157	723.585	262802.	-431.583	127.0316
950.	489.498	749.962	287195.	-447.651	127.1952
1000.	492.389	775.145	311744.	-463.401	127.3595
(2 sigma)	1.770	3.716	379.	3.735	0.1130
1050.	494.913	799.231	336428.	-478.823	127.5243
1100.	497.138	822.307	361231.	-493.915	127.6896
1150.	499.124	844.450	386138.	-508.678	127.8553
1200.	500.920	865.731	411140.	-523.115	128.0214
1250.	502.570	886.213	436228.	-537.231	128.1877
(2 sigma)	3.710	3.748	975.	3.724	0.2297
1300.	504.112	905.955	461395.	-551.036	128.3543
1350.	505.577	925.008	486637.	-564.536	128.5211
1400.	506.996	943.420	511952.	-577.740	128.6881
1450.	508.392	961.236	537337.	-590.659	128.8552
1500.	509.788	978.495	562791.	-603.301	129.0224
(2 sigma)	7.278	3.970	2193.	3.715	0.3627
1550.	511.205	995.234	588316.	-615.675	129.1898
1600.	512.659	1011.487	613912.	-627.791	129.3572
1650.	514.167	1027.285	639583.	-639.659	129.5248
1700.	515.743	1042.657	665330.	-651.287	129.6924
1750.	517.399	1057.631	691158.	-662.684	129.8600
(2 sigma)	12.727	4.675	4510.	3.723	0.5021
1800.	519.147	1072.231	717072.	-673.858	130.0277
(2 sigma)	14.052	4.903	5149.	3.730	0.5304

Table 85. Thermochemical properties of grossular, $Ca_3Al_2Si_3O_{12}$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-6632735.	-6395616.	1670.362	-324725.	-319023.	83.320
250.	-6636790.	-6335822.	1323.797	-325399.	-317518.	66.342
(2 sigma)	---	---	---	4071.	3313.	0.692
273.15	-6638009.	-6307895.	1206.262	-325666.	-316776.	60.577
298.15	-6638943.	-6277637.	1099.815	-325915.	-315951.	55.353
(2 sigma)	---	---	---	4071.	3178.	0.557
300.	-6638998.	-6275395.	1092.643	-325931.	-315889.	55.001
350.	-6639850.	-6214711.	927.494	-326316.	-314183.	46.889
400.	-6639713.	-6153976.	803.626	-326600.	-312430.	40.799
450.	-6638863.	-6093304.	707.292	-326838.	-310644.	36.059
500.	-6637513.	-6032755.	630.237	-327080.	-308832.	32.263
(2 sigma)	---	---	---	4072.	2670.	0.279
550.	-6635829.	-5972359.	567.207	-327368.	-306994.	29.156
600.	-6633945.	-5912125.	514.696	-327738.	-305126.	26.564
650.	-6631968.	-5852053.	470.276	-328219.	-303223.	24.367
700.	-6629987.	-5792135.	432.214	-328836.	-301278.	22.482
750.	-6630583.	-5732246.	399.229	-329607.	-299284.	20.844
(2 sigma)	---	---	---	4066.	2244.	0.156
800.	-6628478.	-5672427.	370.371	-330548.	-297232.	19.407
850.	-6626660.	-5612731.	344.916	-333807.	-295101.	18.135
900.	-6625162.	-5553133.	322.295	-333852.	-292823.	16.995
950.	-6645274.	-5492961.	302.024	-333899.	-290542.	15.975
1000.	-6644230.	-5432341.	283.756	-333962.	-288259.	15.057
(2 sigma)	---	---	---	4055.	2164.	0.113
1050.	-6643463.	-5371767.	267.231	-334052.	-285972.	14.226
1100.	-6642982.	-5311222.	252.209	-334180.	-283679.	13.471
1150.	-6666410.	-5249852.	238.456	-334352.	-281380.	12.781
1200.	-6663694.	-5188321.	225.842	-334575.	-279072.	12.148
1250.	-6660969.	-5126903.	214.241	-334852.	-276754.	11.565
(2 sigma)	---	---	---	4097.	2462.	0.103
1300.	-6658238.	-5065594.	203.538	-335188.	-274424.	11.026
1350.	-6655498.	-5004391.	193.631	-335584.	-272080.	10.527
1400.	-6652749.	-4943289.	184.436	-336041.	-269719.	10.063
1450.	-6649987.	-4882285.	175.879	-336560.	-267342.	9.631
1500.	-6647208.	-4821377.	167.895	-337141.	-264945.	9.226
(2 sigma)	---	---	---	4461.	3036.	0.106
1550.	-6644408.	-4760562.	160.430	-337783.	-262528.	8.847
1600.	-6641580.	-4699838.	153.434	-338484.	-260090.	8.491
1650.	-6638719.	-4639203.	146.865	-339242.	-257628.	8.156
1700.	-6787344.	-4577306.	140.643	-340055.	-255143.	7.840
1750.	-6783967.	-4512353.	134.686	-340919.	-252633.	7.541
(2 sigma)	---	---	---	5862.	3814.	0.114
1800.	-7239023.	-4435728.	128.721	-341833.	-250098.	7.258
(2 sigma)	---	---	---	6347.	3996.	0.116

Table 86. Thermophysical values for hatrurite, Ca_3SiO_5, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	135.792	106.976	-15266.	-183.305	72.7052
250.	156.756	139.661	-7923.	-171.352	72.7213
(2 sigma)	0.547	0.345	33.	0.321	0.5146
273.15	164.422	153.885	-4203.	-169.273	72.7306
298.15	171.658	168.604	0.	-168.604	72.7420
(2 sigma)	0.880	0.321	0.	0.321	0.5144
300.	172.157	169.667	318.	-168.607	72.7429
350.	184.064	197.136	9235.	-170.749	72.7692
400.	193.607	222.359	18685.	-175.646	72.7994
450.	201.463	245.630	28568.	-182.146	72.8331
500.	208.066	267.208	38811.	-189.586	72.8695
(2 sigma)	1.547	0.706	261.	0.340	0.5153
550.	213.707	287.310	49359.	-197.567	72.9084
600.	218.592	306.119	60169.	-205.838	72.9493
650.	222.868	323.788	71208.	-214.238	72.9919
700.	226.647	340.446	82447.	-222.664	73.0360
750.	230.012	356.200	93865.	-231.046	73.0813
(2 sigma)	2.608	1.271	667.	0.493	0.5157
800.	233.030	371.142	105443.	-239.339	73.1276
850.	235.753	385.353	117164.	-247.513	73.1749
900.	238.221	398.899	129014.	-255.550	73.2229
950.	240.469	411.840	140982.	-263.438	73.2715
1000.	242.525	424.228	153058.	-271.170	73.3206
(2 sigma)	4.951	1.969	1416.	0.710	0.5164
1050.	244.412	436.107	165232.	-278.743	73.3703
1100.	246.150	447.518	177496.	-286.157	73.4203
1150.	247.754	458.495	189844.	-293.413	73.4706
1200.	249.239	469.071	202270.	-300.513	73.5212
1250.	250.617	479.274	214767.	-307.461	73.5720
(2 sigma)	7.861	3.076	2855.	0.991	0.5197
1300.	251.898	489.129	227330.	-314.260	73.6230
1350.	253.092	498.658	239955.	-320.914	73.6742
1400.	254.206	507.883	252638.	-327.427	73.7256
1450.	255.247	516.822	265374.	-333.805	73.7770
1500.	256.221	525.491	278161.	-340.051	73.8286
(2 sigma)	11.041	4.574	5100.	1.380	0.5266
1550.	257.134	533.908	290995.	-346.169	73.8802
1600.	257.991	542.085	303874.	-352.164	73.9319
1650.	258.795	550.037	316794.	-358.040	73.9837
1700.	259.551	557.774	329752.	-363.802	74.0356
1750.	260.263	565.308	342748.	-369.452	74.0874
(2 sigma)	14.375	6.375	8188.	1.892	0.5374
1800.	260.932	572.649	355778.	-374.995	74.1393
(2 sigma)	15.055	6.764	8909.	2.009	0.5399

Table 87. Thermochemical properties of hatrurite, Ca_3SiO_5, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

T	Formation from the Elements			Formation from the Oxides		
K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-2932681.	-2836063.	740.703	-117839.	-120324.	31.425
250.	-2933550.	-2811790.	587.491	-117776.	-120955.	25.272
(2 sigma)	---	---	---	1689.	1689.	0.353
273.15	-2933694.	-2800507.	535.542	-117765.	-121250.	23.187
298.15	-2933704.	-2788316.	488.501	-117754.	-121569.	21.298
(2 sigma)	---	---	---	1692.	1690.	0.296
300.	-2933700.	-2787414.	485.331	-117753.	-121593.	21.171
350.	-2933347.	-2763055.	412.363	-117721.	-122235.	18.243
400.	-2932640.	-2738772.	357.647	-117667.	-122883.	16.047
450.	-2931688.	-2714594.	315.102	-117589.	-123540.	14.340
500.	-2930576.	-2690531.	281.078	-117490.	-124206.	12.976
(2 sigma)	---	---	---	1810.	1672.	0.175
550.	-2929368.	-2666584.	253.251	-117374.	-124883.	11.860
600.	-2928117.	-2642749.	230.072	-117248.	-125571.	10.932
650.	-2926866.	-2619020.	210.467	-117117.	-126270.	10.147
700.	-2925651.	-2595385.	193.670	-116987.	-126979.	9.475
750.	-2927013.	-2571726.	179.111	-116862.	-127697.	8.894
(2 sigma)	---	---	---	2211.	1566.	0.109
800.	-2925634.	-2548086.	166.373	-116746.	-128423.	8.385
850.	-2924475.	-2524526.	155.138	-117357.	-129151.	7.937
900.	-2923545.	-2501027.	145.156	-116852.	-129859.	7.537
950.	-2922854.	-2477574.	136.226	-116303.	-130597.	7.181
1000.	-2922407.	-2454151.	128.192	-115717.	-131364.	6.862
(2 sigma)	---	---	---	2945.	1344.	0.070
1050.	-2922212.	-2430744.	120.923	-115100.	-132161.	6.575
1100.	-2922273.	-2407341.	114.315	-114458.	-132989.	6.315
1150.	-2946211.	-2383087.	108.243	-113795.	-133846.	6.079
1200.	-2943971.	-2358651.	102.669	-113117.	-134732.	5.865
1250.	-2941690.	-2334310.	97.545	-112428.	-135647.	5.668
(2 sigma)	---	---	---	4251.	1067.	0.045
1300.	-2939372.	-2310060.	92.819	-111731.	-136589.	5.488
1350.	-2937017.	-2285901.	88.447	-111032.	-137559.	5.322
1400.	-2934630.	-2261829.	84.390	-110333.	-138554.	5.170
1450.	-2932211.	-2237843.	80.616	-109639.	-139574.	5.028
1500.	-2929763.	-2213941.	77.096	-108953.	-140618.	4.897
(2 sigma)	---	---	---	6344.	1199.	0.042
1550.	-2927286.	-2190121.	73.807	-108278.	-141685.	4.775
1600.	-2924782.	-2166381.	70.725	-107617.	-142773.	4.661
1650.	-2922252.	-2142720.	67.833	-106973.	-143881.	4.555
1700.	-2970207.	-2118686.	65.099	-106349.	-145009.	4.456
1750.	-2967485.	-2093681.	62.493	-105749.	-146155.	4.362
(2 sigma)	---	---	---	9310.	2204.	0.066
1800.	-3423238.	-2056983.	59.692	-105175.	-147318.	4.275
(2 sigma)	---	---	---	10010.	2494.	0.072

Table 88. Thermophysical values for rankinite, $Ca_3Si_2O_7$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	167.933	133.933	-18983.	-228.847	96.4050
250.	194.970	174.476	-9873.	-213.969	96.4535
(2 sigma)	0.522	3.095	30.	3.091	0.2582
273.15	204.896	192.186	-5242.	-211.377	96.4770
298.15	214.259	210.543	0.	-210.543	96.5030
(2 sigma)	0.758	3.092	0.	3.092	0.2572
300.	214.903	211.870	397.	-210.547	96.5050
350.	230.239	246.198	11541.	-213.223	96.5590
400.	242.407	277.766	23368.	-219.345	96.6151
450.	252.284	306.906	35744.	-227.476	96.6731
500.	260.443	333.923	48568.	-236.786	96.7326
(2 sigma)	1.511	3.122	225.	3.090	0.2619
550.	267.276	359.075	61766.	-246.773	96.7934
600.	273.060	382.586	75278.	-257.122	96.8553
650.	277.996	404.643	89058.	-267.630	96.9181
700.	282.238	425.403	103066.	-278.166	96.9817
750.	285.901	445.004	117272.	-288.641	97.0460
(2 sigma)	1.707	3.259	611.	3.099	0.2636
800.	289.076	463.559	131648.	-298.999	97.1109
850.	291.835	481.169	146173.	-309.201	97.1762
900.	294.236	497.919	160826.	-319.224	97.2420
950.	296.327	513.885	175591.	-329.052	97.3081
1000.	298.146	529.132	190454.	-338.678	97.3745
(2 sigma)	2.046	3.390	957.	3.126	0.2659
1050.	299.726	543.718	205402.	-348.097	97.4411
1100.	301.095	557.694	220423.	-357.309	97.5079
1150.	302.275	571.105	235508.	-366.315	97.5750
1200.	303.285	583.991	250648.	-375.118	97.6421
1250.	304.144	596.390	265834.	-383.722	97.7094
(2 sigma)	3.560	3.495	1343.	3.160	0.2784
1300.	304.866	608.333	281060.	-392.133	97.7768
1350.	305.463	619.850	296319.	-400.355	97.8443
1400.	305.946	630.968	311604.	-408.394	97.9119
1450.	306.326	641.711	326912.	-416.255	97.9795
1500.	306.612	652.101	342235.	-423.944	98.0472
(2 sigma)	5.811	3.683	2143.	3.193	0.3043
1550.	306.810	662.158	357571.	-431.467	98.1149
1600.	306.927	671.901	372915.	-438.829	98.1827
1650.	306.971	681.347	388263.	-446.036	98.2505
(2 sigma)	7.404	3.955	3092.	3.218	0.3274

Table 89. Thermochemical properties of rankinite, $Ca_3Si_2O_7$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-3973107.	-3840871.	1003.132	-248386.	-251058.	65.570
250.	-3974516.	-3807628.	795.560	-248369.	-251730.	52.596
(2 sigma)	---	---	---	3366.	2715.	0.567
273.15	-3974857.	-3792158.	725.176	-248392.	-252041.	48.198
298.15	-3975050.	-3775426.	661.439	-248429.	-252373.	44.215
(2 sigma)	---	---	---	3368.	2597.	0.455
300.	-3975057.	-3774188.	657.144	-248432.	-252398.	43.946
350.	-3974990.	-3740708.	558.270	-248534.	-253051.	37.766
400.	-3974494.	-3707268.	484.119	-248667.	-253687.	33.128
450.	-3973705.	-3673910.	426.456	-248837.	-254305.	29.519
500.	-3972722.	-3640651.	380.336	-249055.	-254902.	26.629
(2 sigma)	---	---	---	3404.	2133.	0.223
550.	-3971625.	-3607496.	342.611	-249331.	-255473.	24.263
600.	-3970478.	-3574444.	311.183	-249674.	-256017.	22.288
650.	-3969333.	-3541488.	284.597	-250095.	-256529.	20.615
700.	-3968234.	-3508618.	261.816	-250602.	-257006.	19.178
750.	-3969725.	-3475715.	242.070	-251202.	-257443.	17.930
(2 sigma)	---	---	---	3497.	1675.	0.117
800.	-3968496.	-3442822.	224.793	-251904.	-257837.	16.835
850.	-3967510.	-3409999.	209.553	-254138.	-258173.	15.865
900.	-3966782.	-3377227.	196.009	-254214.	-258408.	14.998
950.	-3966322.	-3344487.	183.893	-254278.	-258639.	14.221
1000.	-3966140.	-3311765.	172.989	-254340.	-258867.	13.522
(2 sigma)	---	---	---	3602.	1523.	0.080
1050.	-3966245.	-3279045.	163.123	-254410.	-259092.	12.889
1100.	-3966643.	-3246313.	154.154	-254496.	-259313.	12.314
1150.	-3990957.	-3212715.	145.926	-254607.	-259529.	11.788
1200.	-3989133.	-3178918.	138.375	-254750.	-259740.	11.306
1250.	-3987309.	-3145196.	131.430	-254932.	-259944.	10.862
(2 sigma)	---	---	---	3716.	1808.	0.076
1300.	-3985491.	-3111548.	125.023	-255158.	-260141.	10.453
1350.	-3983679.	-3077969.	119.094	-255436.	-260327.	10.073
1400.	-3981879.	-3044457.	113.590	-255771.	-260502.	9.719
1450.	-3980093.	-3011009.	108.468	-256167.	-260665.	9.390
1500.	-3978322.	-2977623.	103.690	-256630.	-260812.	9.082
(2 sigma)	---	---	---	4028.	2404.	0.084
1550.	-3976569.	-2944295.	99.222	-257164.	-260943.	8.794
1600.	-3974835.	-2911024.	95.035	-257773.	-261055.	8.523
1650.	-3973122.	-2877806.	91.104	-258463.	-261147.	8.267
(2 sigma)	---	---	---	4614.	2876.	0.091

Table 90. Thermophysical values for meionite, $Ca_4Al_6Si_6O_{24}(CO_3)$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	466.964	450.253	-60109.	-750.796	337.0425
250.	623.750	572.781	-32508.	-702.815	337.3241
(2 sigma)	20.017	12.267	684.	11.982	2.1893
273.15	674.831	630.323	-17458.	-694.236	337.4544
298.15	720.385	691.450	0.	-691.450	337.5952
(2 sigma)	10.808	12.002	0.	12.002	2.0810
300.	723.434	695.915	1336.	-691.463	337.6056
350.	793.116	812.953	39342.	-700.546	337.8872
400.	845.051	922.404	80354.	-721.518	338.1687
450.	885.571	1024.367	123659.	-749.570	338.4503
500.	918.281	1119.421	168782.	-781.857	338.7319
(2 sigma)	11.223	8.118	1997.	11.184	1.6348
550.	945.390	1208.252	215394.	-816.627	339.0134
600.	968.325	1291.521	263252.	-852.768	339.2950
650.	988.058	1369.827	312173.	-889.560	339.5766
700.	1005.271	1443.693	362016.	-926.528	339.8581
750.	1020.460	1513.578	412666.	-963.356	340.1397
(2 sigma)	8.890	5.199	4377.	9.411	1.1179
800.	1033.994	1579.877	464034.	-999.835	340.4212
850.	1046.155	1642.934	516043.	-1035.825	340.7028
900.	1057.161	1703.047	568630.	-1071.236	340.9844
950.	1067.186	1760.478	621743.	-1106.012	341.2659
1000.	1076.368	1815.454	675335.	-1140.119	341.5475
(2 sigma)	7.320	4.229	6072.	7.917	0.7244
1050.	1084.819	1868.177	729367.	-1173.542	341.8291
1100.	1092.633	1918.826	783806.	-1206.275	342.1106
1150.	1099.886	1967.557	838621.	-1238.321	342.3922
1200.	1106.643	2014.513	893787.	-1269.690	342.6737
1250.	1112.958	2059.817	949278.	-1300.395	342.9553
(2 sigma)	7.837	4.162	7284.	6.816	0.7055
1300.	1118.878	2103.585	1005076.	-1330.450	343.2369
1350.	1124.443	2145.917	1061160.	-1359.873	343.5184
1400.	1129.686	2186.906	1117515.	-1388.681	343.8000
1450.	1134.639	2226.636	1174124.	-1416.895	344.0816
1500.	1139.327	2265.181	1230974.	-1444.532	344.3631
(2 sigma)	9.390	4.658	8386.	6.041	1.0810
1550.	1143.772	2302.613	1288053.	-1471.611	344.6447
1600.	1147.996	2338.993	1345348.	-1498.151	344.9263
1650.	1152.017	2374.381	1402849.	-1524.170	345.2078
1700.	1155.849	2408.830	1460546.	-1549.685	345.4894
1750.	1159.508	2442.388	1518431.	-1574.713	345.7709
(2 sigma)	11.140	5.545	9724.	5.528	1.5929
1800.	1163.007	2475.102	1576495.	-1599.272	346.0525
(2 sigma)	11.483	5.756	10042.	5.453	1.7014

Table 91. Thermochemical properties of meionite, $Ca_4Al_6Si_6O_{24}(CO_3)$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-13884220.	-13389268.	3496.916	-471259.	-456964.	119.347
250.	-13893419.	-13264332.	2771.429	-472450.	-453209.	94.693
(2 sigma)	---	---	---	8922.	6463.	1.350
273.15	-13895848.	-13205962.	2525.382	-472475.	-451425.	86.326
298.15	-13897549.	-13142738.	2302.552	-472316.	-449504.	78.751
(2 sigma)	---	---	---	8939.	6043.	1.059
300.	-13897643.	-13138055.	2287.537	-472298.	-449363.	78.241
350.	-13898807.	-13011331.	1941.833	-471690.	-445585.	66.500
400.	-13897964.	-12884587.	1682.553	-471012.	-441903.	57.707
450.	-13895762.	-12758035.	1480.913	-470449.	-438300.	50.876
500.	-13892631.	-12631782.	1319.632	-470093.	-434749.	45.418
(2 sigma)	---	---	---	7793.	4725.	0.494
550.	-13888876.	-12505874.	1187.708	-469991.	-431222.	40.954
600.	-13884727.	-12380328.	1077.803	-470165.	-427692.	37.234
650.	-13880359.	-12255137.	984.834	-470628.	-424135.	34.084
700.	-13875914.	-12130287.	905.172	-471384.	-420533.	31.380
750.	-13874855.	-12005607.	836.144	-472434.	-416865.	29.033
(2 sigma)	---	---	---	6494.	3949.	0.275
800.	-13870157.	-11881146.	775.759	-473780.	-413119.	26.974
850.	-13865821.	-11756968.	722.495	-479694.	-409247.	25.149
900.	-13861908.	-11633033.	675.163	-479089.	-405120.	23.513
950.	-13922247.	-11507360.	632.718	-478382.	-401030.	22.050
1000.	-13918520.	-11380358.	594.449	-477592.	-396978.	20.736
(2 sigma)	---	---	---	5882.	3665.	0.191
1050.	-13915006.	-11253538.	559.832	-476734.	-392969.	19.549
1100.	-13911723.	-11126879.	528.371	-475821.	-389001.	18.472
1150.	-13940172.	-10999243.	499.601	-474867.	-385076.	17.491
1200.	-13933620.	-10871516.	473.224	-473885.	-381193.	16.593
1250.	-13926922.	-10744066.	448.970	-472886.	-377351.	15.769
(2 sigma)	---	---	---	5838.	3702.	0.155
1300.	-13920086.	-10616886.	426.591	-471883.	-373550.	15.009
1350.	-13913118.	-10489972.	405.881	-470887.	-369787.	14.308
1400.	-13906024.	-10363318.	386.660	-469907.	-366060.	13.658
1450.	-13898808.	-10236920.	368.773	-468955.	-362368.	13.054
1500.	-13891473.	-10110772.	352.088	-468042.	-358708.	12.491
(2 sigma)	---	---	---	6472.	4029.	0.140
1550.	-13884020.	-9984871.	336.488	-467177.	-355078.	11.966
1600.	-13876452.	-9859213.	321.870	-466370.	-351475.	11.474
1650.	-13868770.	-9733793.	308.146	-465632.	-347897.	11.013
1700.	-14164029.	-9605908.	295.153	-464972.	-344339.	10.580
1750.	-14155267.	-9471973.	282.723	-464400.	-340799.	10.172
(2 sigma)	---	---	---	7913.	4673.	0.139
1800.	-14757700.	-9322595.	270.534	-463925.	-337275.	9.787
(2 sigma)	---	---	---	8297.	4844.	0.141

Table 92. Thermophysical values for stable phases of the element iron (Fe) at 1.01325 bars (1 atm). Lambda transition occurs at 1042 K. The sources of data are given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
	iron (crystal, body centered cubic)				
200.	34.683	16.270	-2677.	-29.652	---
250.	26.027	22.838	-1213.	-27.688	---
(2 sigma)	---	---	---	---	---
273.15	25.059	25.093	-623.	-27.375	---
298.15	24.925	27.276	-0.	-27.276	---
(2 sigma)	---	---	---	---	---
300.	24.939	27.431	46.	-27.277	---
350.	25.946	31.339	1314.	-27.583	---
400.	27.366	34.896	2647.	-28.278	---
450.	28.704	38.198	4050.	-29.199	---
500.	29.872	41.284	5515.	-30.255	---
(2 sigma)	---	---	---	---	---
550.	30.926	44.181	7035.	-31.391	---
600.	31.966	46.916	8607.	-32.571	---
650.	33.097	49.519	10233.	-33.776	---
700.	34.419	52.018	11920.	-34.990	---
750.	36.021	54.446	13679.	-36.206	---
(2 sigma)	---	---	---	---	---
800.	37.980	56.831	15528.	-37.421	---
850.	40.362	59.203	17485.	-38.633	---
900.	43.225	61.588	19572.	-39.842	---
950.	46.617	64.014	21816.	-41.050	---
1000.	50.581	66.503	24243.	-42.260	---
(2 sigma)	---	---	---	---	---
1042.	84.	69.21	26980.	-43.32	---
1050.	51.421	69.706	27537.	-43.480	---
1100.	46.636	71.981	29982.	-44.725	---
1150.	43.281	73.976	32225.	-45.954	---
1184.	41.640	75.212	33667.	-46.777	---
	iron (crystal, face centered cubic)				
1184.	33.882	75.975	34570.	-46.777	---
1200.	34.016	76.430	35113.	-47.169	---
1250.	34.434	77.827	36824.	-48.368	---
(2 sigma)	---	---	---	---	---
1300.	34.853	79.186	38557.	-49.527	---
1350.	35.271	80.509	40310.	-50.650	---
1400.	35.690	81.799	42084.	-51.740	---
1450.	36.108	83.059	43879.	-52.798	---
1500.	36.526	84.290	45694.	-53.827	---
(2 sigma)	---	---	---	---	---
1550.	36.945	85.495	47531.	-54.830	---
1600.	37.363	86.674	49389.	-55.806	---
1650.	37.782	87.831	51268.	-56.759	---
1665.	37.907	88.173	51835.	-57.041	---
	iron (crystal, body centered cubic)				
1665.	41.188	88.666	52656.	-57.040	---
1700.	41.620	89.527	54105.	-57.700	---
1750.	42.204	90.742	56201.	-58.627	---
(2 sigma)	---	---	---	---	---
1800.	42.732	91.939	58325.	-59.536	---
(2 sigma)	---	---	---	---	---

Table 93. Thermochemical properties of stable phases of the element iron (Fe) at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
	iron (crystal, body centered cubic)					
200.	0.	0.	0.	---	---	---
250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
273.15	0.	0.	0.	---	---	---
298.15	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
300.	0.	0.	0.	---	---	---
350.	0.	0.	0.	---	---	---
400.	0.	0.	0.	---	---	---
450.	0.	0.	0.	---	---	---
500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
550.	0.	0.	0.	---	---	---
600.	0.	0.	0.	---	---	---
650.	0.	0.	0.	---	---	---
700.	0.	0.	0.	---	---	---
750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
800.	0.	0.	0.	---	---	---
850.	0.	0.	0.	---	---	---
900.	0.	0.	0.	---	---	---
950.	0.	0.	0.	---	---	---
1000.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1042.	0.	0.	0.	---	---	---
1050.	0.	0.	0.	---	---	---
1100.	0.	0.	0.	---	---	---
1150.	0.	0.	0.	---	---	---
1184.	0.	0.	0.	---	---	---
	iron (crystal, face centered cubic)					
1184.	0.	0.	0.	---	---	---
1200.	0.	0.	0.	---	---	---
1250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1300.	0.	0.	0.	---	---	---
1350.	0.	0.	0.	---	---	---
1400.	0.	0.	0.	---	---	---
1450.	0.	0.	0.	---	---	---
1500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1550.	0.	0.	0.	---	---	---
1600.	0.	0.	0.	---	---	---
1650.	0.	0.	0.	---	---	---
1665.	0.	0.	0.	---	---	---
	iron (crystal, body centered cubic)					
1665.	0.	0.	0.	---	---	---
1700.	0.	0.	0.	---	---	---
1750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1800.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---

Table 94. Thermophysical values for wustite, $Fe_{.947}O$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm^3/mol
200.	44.634	39.849	-4587.	-62.785	12.0395
250.	46.879	50.066	-2296.	-59.249	12.0395
(2 sigma)	0.244	0.565	10.	0.563	0.0053
273.15	47.671	54.253	-1201.	-58.650	12.0395
298.15	48.402	58.460	0.	-58.460	12.0395
(2 sigma)	0.207	0.563	0.	0.563	0.0053
300.	48.452	58.760	90.	-58.461	12.0395
350.	49.619	66.320	2543.	-59.056	12.0395
400.	50.524	73.008	5047.	-60.390	12.0395
450.	51.256	79.002	7592.	-62.130	12.0395
500.	51.870	84.435	10171.	-64.093	12.0395
(2 sigma)	0.208	0.560	42.	0.561	0.0053
550.	52.403	89.404	12778.	-66.172	12.0395
600.	52.883	93.985	15410.	-68.301	12.0395
650.	53.327	98.235	18066.	-70.442	12.0395
700.	53.750	102.203	20743.	-72.571	12.0395
750.	54.164	105.926	23440.	-74.672	12.0395
(2 sigma)	0.311	0.548	79.	0.556	0.0053
800.	54.576	109.434	26159.	-76.736	12.0395
850.	54.994	112.756	28898.	-78.758	12.0395
900.	55.422	115.911	31659.	-80.735	12.0395
950.	55.865	118.919	34441.	-82.666	12.0395
1000.	56.327	121.796	37245.	-84.551	12.0395
(2 sigma)	0.320	0.541	128.	0.550	0.0053
1050.	56.810	124.556	40074.	-86.391	12.0395
1100.	57.317	127.211	42927.	-88.186	12.0395
1150.	57.851	129.770	45806.	-89.939	12.0395
1200.	58.412	132.244	48712.	-91.650	12.0395
1250.	59.003	134.640	51648.	-93.322	12.0395
(2 sigma)	0.615	0.539	151.	0.545	0.0053
1300.	59.625	136.967	54613.	-94.956	12.0395
1350.	60.279	139.229	57611.	-96.554	12.0395
1400.	60.965	141.433	60641.	-98.118	12.0395
1450.	61.686	143.585	63708.	-99.649	12.0395
1500.	62.442	145.689	66811.	-101.149	12.0395
(2 sigma)	1.702	0.571	293.	0.543	0.0053
1550.	63.233	147.749	69952.	-102.619	12.0395
1600.	64.060	149.770	73135.	-104.061	12.0395
1650.	64.923	151.754	76359.	-105.476	12.0395
1700.	65.824	153.706	79627.	-106.866	12.0395
1750.	66.762	155.627	82942.	-108.232	12.0395
(2 sigma)	3.433	0.780	869.	0.545	0.0053
1800.	67.738	157.522	86304.	-109.575	12.0395
(2 sigma)	3.854	0.856	1045.	0.547	0.0053

Table 95. Thermochemical properties of wustite, $Fe_{.947}O$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements. The properties relative to the oxides were unavailable. Refer to Section 1.5.5 for details.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-266038.	-251586.	65.708	---	---	---
250.	-265860.	-247984.	51.813	---	---	---
(2 sigma)	621.	492.	0.103	---	---	---
273.15	-265661.	-246337.	47.107	---	---	---
298.15	-265416.	-244579.	42.849	---	---	---
(2 sigma)	621.	468.	0.082	---	---	---
300.	-265397.	-244450.	42.562	---	---	---
350.	-264885.	-240999.	35.967	---	---	---
400.	-264395.	-237621.	31.030	---	---	---
450.	-263942.	-234301.	27.197	---	---	---
500.	-263527.	-231031.	24.136	---	---	---
(2 sigma)	622.	371.	0.039	---	---	---
550.	-263147.	-227800.	21.635	---	---	---
600.	-262802.	-224602.	19.553	---	---	---
650.	-262495.	-221431.	17.794	---	---	---
700.	-262234.	-218283.	16.288	---	---	---
750.	-262030.	-215151.	14.984	---	---	---
(2 sigma)	618.	267.	0.019	---	---	---
800.	-261898.	-212030.	13.844	---	---	---
850.	-261855.	-208915.	12.838	---	---	---
900.	-261924.	-205800.	11.944	---	---	---
950.	-262125.	-202677.	11.144	---	---	---
1000.	-262485.	-199540.	10.423	---	---	---
(2 sigma)	614.	208.	0.011	---	---	---
1050.	-263647.	-196375.	9.769	---	---	---
1100.	-263987.	-193163.	9.173	---	---	---
1150.	-264114.	-189940.	8.627	---	---	---
1200.	-264831.	-186704.	8.127	---	---	---
1250.	-264409.	-183458.	7.666	---	---	---
(2 sigma)	613.	226.	0.009	---	---	---
1300.	-263981.	-180228.	7.242	---	---	---
1350.	-263545.	-177015.	6.849	---	---	---
1400.	-263098.	-173818.	6.485	---	---	---
1450.	-262640.	-170638.	6.147	---	---	---
1500.	-262167.	-167473.	5.832	---	---	---
(2 sigma)	673.	308.	0.011	---	---	---
1550.	-261679.	-164325.	5.538	---	---	---
1600.	-261172.	-161192.	5.262	---	---	---
1650.	-260644.	-158076.	5.004	---	---	---
1700.	-260983.	-154959.	4.761	---	---	---
1750.	-260575.	-151847.	4.532	---	---	---
(2 sigma)	1084.	429.	0.013	---	---	---
1800.	-260146.	-148746.	4.317	---	---	---
(2 sigma)	1236.	459.	0.013	---	---	---

Table 96. Thermophysical values for ferrosilite, $FeSiO_3$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T	C_p°	S°	$H_T^\circ - H_{298}^\circ$	$[G_T^\circ - H_{298}^\circ]/T$	V°
K	J/(mol K)	J/(mol K)	J/mol	J/(mol K)	cm3/mol
200.	41.873	69.753	-6577.	-102.635	32.8694
250.	69.252	82.360	-3726.	-97.265	32.9300
(2 sigma)	5.802	2.358	201.	2.232	0.0376
273.15	77.404	88.863	-2025.	-96.276	32.9580
298.15	84.327	95.952	0.	-95.952	32.9883
(2 sigma)	3.005	2.235	0.	2.235	0.0352
300.	84.778	96.475	156.	-95.954	32.9906
350.	94.685	110.339	4659.	-97.026	33.0511
400.	101.577	123.457	9575.	-99.518	33.1117
450.	106.696	135.730	14788.	-102.868	33.1722
500.	110.699	147.187	20226.	-106.734	33.2328
(2 sigma)	2.137	1.667	381.	2.105	0.0310
550.	113.956	157.895	25845.	-110.903	33.2933
600.	116.691	167.931	31613.	-115.242	33.3539
650.	119.046	177.366	37508.	-119.661	33.4145
700.	121.114	186.266	43513.	-124.104	33.4750
750.	122.955	194.686	49616.	-128.531	33.5356
(2 sigma)	1.681	1.316	791.	1.832	0.0405
800.	124.616	202.675	55806.	-132.918	33.5961
850.	126.126	210.276	62075.	-137.246	33.6567
900.	127.509	217.525	68416.	-141.506	33.7173
950.	128.782	224.453	74824.	-145.691	33.7778
1000.	129.957	231.089	81293.	-149.796	33.8384
(2 sigma)	1.651	1.291	1064.	1.627	0.0588
1050.	131.045	237.456	87818.	-153.820	33.8989
1100.	132.053	243.576	94396.	-157.762	33.9595
1150.	132.987	249.467	101022.	-161.622	34.0200
1200.	133.853	255.146	107694.	-165.401	34.0806
1250.	134.653	260.626	114407.	-169.101	34.1412
(2 sigma)	1.842	1.401	1282.	1.503	0.0800
1300.	135.391	265.922	121158.	-172.723	34.2017
1350.	136.070	271.044	127945.	-176.271	34.2623
1400.	136.692	276.004	134764.	-179.744	34.3228
1450.	137.258	280.811	141613.	-183.147	34.3834
1500.	137.770	285.473	148489.	-186.481	34.4440
(2 sigma)	1.750	1.556	1511.	1.440	0.1024
1550.	138.230	289.998	155389.	-189.747	34.5045
1600.	138.637	294.394	162311.	-192.949	34.5651
1650.	138.994	298.665	169252.	-196.088	34.6256
1700.	139.301	302.819	176210.	-199.167	34.6862
1750.	139.558	306.861	183181.	-202.186	34.7467
(2 sigma)	1.912	1.675	1716.	1.418	0.1253
1800.	139.767	310.796	190165.	-205.149	34.8073
(2 sigma)	2.095	1.691	1752.	1.417	0.1299

Table 97. Thermochemical properties of ferrosilite, $FeSiO_3$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements. The properties relative to the oxides were unavailable. Refer to Section 1.5.5 for details.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-1192120.	-1142467.	298.382	---	---	---
250.	-1193767.	-1129829.	236.065	---	---	---
(2 sigma)	1457.	961.	0.201	---	---	---
273.15	-1194100.	-1123892.	214.922	---	---	---
298.15	-1194286.	-1117457.	195.774	---	---	---
(2 sigma)	1460.	875.	0.153	---	---	---
300.	-1194294.	-1116981.	194.483	---	---	---
350.	-1194312.	-1104089.	164.776	---	---	---
400.	-1194069.	-1091214.	142.498	---	---	---
450.	-1193678.	-1078379.	125.175	---	---	---
500.	-1193191.	-1065594.	111.322	---	---	---
(2 sigma)	1283.	585.	0.061	---	---	---
550.	-1192641.	-1052860.	99.992	---	---	---
600.	-1192050.	-1040179.	90.556	---	---	---
650.	-1191437.	-1027548.	82.575	---	---	---
700.	-1190821.	-1014964.	75.737	---	---	---
750.	-1190223.	-1002424.	69.815	---	---	---
(2 sigma)	1077.	458.	0.032	---	---	---
800.	-1189666.	-989922.	64.635	---	---	---
850.	-1189175.	-977454.	60.067	---	---	---
900.	-1188777.	-965012.	56.008	---	---	---
950.	-1188500.	-952588.	52.377	---	---	---
1000.	-1188376.	-940176.	49.110	---	---	---
(2 sigma)	1014.	579.	0.030	---	---	---
1050.	-1189090.	-927760.	46.154	---	---	---
1100.	-1188928.	-915319.	43.465	---	---	---
1150.	-1188540.	-902890.	41.011	---	---	---
1200.	-1188776.	-890470.	38.761	---	---	---
1250.	-1187813.	-878061.	36.692	---	---	---
(2 sigma)	1118.	840.	0.035	---	---	---
1300.	-1186853.	-865689.	34.784	---	---	---
1350.	-1185898.	-853355.	33.018	---	---	---
1400.	-1184947.	-841056.	31.380	---	---	---
1450.	-1184004.	-828791.	29.856	---	---	---
1500.	-1183069.	-816558.	28.435	---	---	---
(2 sigma)	1358.	1169.	0.041	---	---	---
1550.	-1182145.	-804356.	27.107	---	---	---
1600.	-1181232.	-792184.	25.862	---	---	---
1650.	-1180332.	-780041.	24.694	---	---	---
1700.	-1230894.	-767456.	23.581	---	---	---
1750.	-1230058.	-753838.	22.501	---	---	---
(2 sigma)	1603.	1542.	0.046	---	---	---
1800.	-1229242.	-740243.	21.481	---	---	---
(2 sigma)	1646.	1620.	0.047	---	---	---

Table 98. Thermophysical values for hematite, Fe_2O_3, at 1.01325 bars (1 atm). Lambda transition occurs at 955.50 K. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T	C_p°	S°	$H_T^\circ - H_{298}^\circ$	$[G_T^\circ - H_{298}^\circ]/T$	V°
K	J/(mol K)	J/(mol K)	J/mol	J/(mol K)	cm3/mol
200.	76.761	51.370	-8965.	-96.193	30.1601
250.	92.138	70.206	-4730.	-89.125	30.2187
(2 sigma)	0.116	0.320	5.	0.319	0.0208
273.15	98.132	78.633	-2526.	-87.880	30.2458
298.15	103.801	87.477	0.	-87.477	30.2751
(2 sigma)	0.109	0.319	0.	0.319	0.0181
300.	104.190	88.121	192.	-87.479	30.2772
350.	113.284	104.897	5640.	-88.783	30.3358
400.	120.215	120.497	11485.	-91.785	30.3944
450.	125.694	134.983	17637.	-95.789	30.4530
500.	130.279	148.470	24039.	-100.391	30.5116
(2 sigma)	0.276	0.332	39.	0.320	0.0346
550.	134.398	161.082	30657.	-105.341	30.5702
600.	138.380	172.947	37477.	-110.485	30.6287
650.	142.478	184.184	44497.	-115.726	30.6873
700.	146.889	194.901	51730.	-121.001	30.7459
750.	151.771	205.199	59194.	-126.273	30.8045
(2 sigma)	0.374	0.370	104.	0.324	0.0719
800.	157.250	215.166	66917.	-131.519	30.8631
850.	163.427	224.880	74931.	-136.726	30.9217
900.	170.385	234.415	83273.	-141.889	30.9802
950.	186.95	243.93	92051.	-147.03	31.0388
955.50	195.42	244.92	92998.	-147.59	31.0453
1000.	150.364	254.002	101851.	-152.150	31.0974
(2 sigma)	0.824	1.247	1179.	0.330	0.1111
1050.	143.691	261.165	109191.	-157.173	31.1560
1100.	139.445	267.743	116261.	-162.052	31.2146
1150.	137.000	273.882	123166.	-166.782	31.2732
1200.	135.880	279.685	129983.	-171.366	31.3317
1250.	135.720	285.226	136770.	-175.811	31.3903
(2 sigma)	2.386	1.254	1201.	0.417	0.1508
1300.	136.238	290.558	143566.	-180.122	31.4489
1350.	137.217	295.716	150401.	-184.308	31.5075
1400.	138.487	300.729	157293.	-188.377	31.5661
1450.	139.919	305.613	164252.	-192.336	31.6247
1500.	141.408	310.382	171286.	-196.192	31.6832
(2 sigma)	2.464	1.368	1420.	0.530	0.1906
1550.	142.876	315.043	178393.	-199.951	31.7418
1600.	144.261	319.601	185572.	-203.619	31.8004
1650.	145.516	324.060	192817.	-207.201	31.8590
1700.	146.603	328.420	200121.	-210.702	31.9176
1750.	147.496	332.684	207474.	-214.127	31.9762
(2 sigma)	2.380	1.509	1731.	0.635	0.2306
1800.	148.173	336.849	214867.	-217.478	32.0347
(2 sigma)	2.297	1.534	1792.	0.655	0.2386

Table 99. Thermochemical properties of hematite, Fe_2O_3, at 1.01325 bars (1 atm). Lambda transition occurs at 955.50 K. Columns 2 through 4 give the thermochemical values relative to the elements. The properties relative to the oxides were unavailable. Refer to Section 1.5.5 for details.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-826468.	-772215.	201.682	---	---	---
250.	-827343.	-758517.	158.483	---	---	---
(2 sigma)	1071.	1043.	0.218	---	---	---
273.15	-827329.	-752143.	143.833	---	---	---
298.15	-827148.	-745269.	130.568	---	---	---
(2 sigma)	1071.	1038.	0.182	---	---	---
300.	-827130.	-744761.	129.674	---	---	---
350.	-826439.	-731083.	109.108	---	---	---
400.	-825515.	-717522.	93.699	---	---	---
450.	-824460.	-704085.	81.728	---	---	---
500.	-823316.	-690770.	72.164	---	---	---
(2 sigma)	1075.	1019.	0.106	---	---	---
550.	-822101.	-677574.	64.351	---	---	---
600.	-820821.	-664491.	57.849	---	---	---
650.	-819478.	-651518.	52.357	---	---	---
700.	-818075.	-638650.	47.657	---	---	---
750.	-816612.	-625884.	43.590	---	---	---
(2 sigma)	1086.	999.	0.070	---	---	---
800.	-815094.	-613218.	40.039	---	---	---
850.	-813526.	-600649.	36.911	---	---	---
900.	-811915.	-588173.	34.137	---	---	---
950.	-810200.	-575808.	31.660	---	---	---
955.50	-810052.	-574451.	31.404	---	---	---
1000.	-807851.	-563557.	29.437	---	---	---
1050.	-809714.	-551322.	27.427	---	---	---
1100.	-810166.	-539006.	25.595	---	---	---
1150.	-810395.	-526675.	23.922	---	---	---
1200.	-812019.	-514315.	22.388	---	---	---
1250.	-811332.	-501925.	20.974	---	---	---
(2 sigma)	2035.	778.	0.032	---	---	---
1300.	-810691.	-489561.	19.671	---	---	---
1350.	-810065.	-477222.	18.465	---	---	---
1400.	-809435.	-464906.	17.346	---	---	---
1450.	-808789.	-452613.	16.305	---	---	---
1500.	-808120.	-440342.	15.334	---	---	---
(2 sigma)	2195.	694.	0.024	---	---	---
1550.	-807427.	-428094.	14.427	---	---	---
1600.	-806712.	-415869.	13.577	---	---	---
1650.	-805978.	-403666.	12.779	---	---	---
1700.	-807109.	-391450.	12.028	---	---	---
1750.	-806712.	-379231.	11.319	---	---	---
(2 sigma)	2419.	766.	0.023	---	---	---
1800.	-806334.	-367023.	10.651	---	---	---
(2 sigma)	2465.	801.	0.023	---	---	---
(2 sigma)	---	---	---	---	---	---

Table 100. Thermophysical values for fayalite, Fe_2SiO_4, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
200.	102.407	104.772	-11594.	-162.740	46.0018
250.	118.884	129.437	-6051.	-153.643	46.0761
(2 sigma)	0.193	1.072	9.	1.072	0.0331
273.15	125.550	140.262	-3221.	-152.053	46.1105
298.15	131.991	151.540	0.	-151.540	46.1477
(2 sigma)	0.167	1.072	0.	1.072	0.0309
300.	132.437	152.358	245.	-151.543	46.1505
350.	143.065	173.606	7143.	-153.196	46.2248
400.	151.318	193.271	14512.	-156.993	46.2991
450.	157.747	211.481	22245.	-162.048	46.3734
500.	162.797	228.373	30263.	-167.846	46.4477
(2 sigma)	0.470	1.079	54.	1.072	0.0224
550.	166.821	244.085	38507.	-174.071	46.5220
600.	170.088	258.745	46933.	-180.524	46.5964
650.	172.811	272.470	55507.	-187.074	46.6707
700.	175.155	285.364	64208.	-193.639	46.7450
750.	177.253	297.521	73019.	-200.163	46.8193
(2 sigma)	0.929	1.121	202.	1.074	0.0171
800.	179.210	309.024	81931.	-206.611	46.8936
850.	181.113	319.945	90939.	-212.959	46.9679
900.	183.033	330.352	100042.	-219.194	47.0423
950.	185.028	340.301	109243.	-225.308	47.1166
1000.	187.147	349.845	118547.	-231.298	47.1909
(2 sigma)	0.990	1.174	360.	1.082	0.0216
1050.	189.431	359.030	127961.	-237.163	47.2652
1100.	191.917	367.899	137493.	-242.905	47.3395
1150.	194.633	376.489	147156.	-248.527	47.4138
1200.	197.605	384.834	156961.	-254.034	47.4882
1250.	200.857	392.966	166921.	-259.429	47.5625
(2 sigma)	4.041	1.176	521.	1.088	0.0321
1300.	204.406	400.912	177052.	-264.718	47.6368
1350.	208.271	408.698	187367.	-269.907	47.7111
1400.	212.466	416.347	197884.	-275.001	47.7854
1450.	217.005	423.881	208620.	-280.005	47.8597
1500.	221.898	431.319	219591.	-284.925	47.9341
(2 sigma)	10.553	1.796	2066.	1.090	0.0445
1550.	227.157	438.680	230815.	-289.766	48.0084
1600.	232.791	445.980	242313.	-294.534	48.0827
1650.	238.808	453.234	254101.	-299.233	48.1570
1700.	245.216	460.457	266200.	-303.869	48.2313
1750.	252.021	467.663	278629.	-308.446	48.3056
(2 sigma)	20.446	3.837	5795.	1.153	0.0576
1800.	259.230	474.863	291409.	-312.969	48.3800
(2 sigma)	22.841	4.415	6865.	1.189	0.0602

Table 101. Thermochemical properties of fayalite, Fe_2SiO_4, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements. The properties relative to the oxides were not available. Refer to Section 1.5.5 for details.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-1477912.	-1412670.	368.951	---	---	---
250.	-1479058.	-1396195.	291.719	---	---	---
(2 sigma)	1381.	1147.	0.240	---	---	---
273.15	-1479189.	-1388515.	265.526	---	---	---
298.15	-1479168.	-1380216.	241.808	---	---	---
(2 sigma)	1380.	1104.	0.193	---	---	---
300.	-1479161.	-1379602.	240.210	---	---	---
350.	-1478792.	-1363033.	203.421	---	---	---
400.	-1478182.	-1346536.	175.839	---	---	---
450.	-1477436.	-1330123.	154.397	---	---	---
500.	-1476611.	-1313799.	137.252	---	---	---
(2 sigma)	1387.	931.	0.097	---	---	---
550.	-1475744.	-1297560.	123.232	---	---	---
600.	-1474866.	-1281400.	111.556	---	---	---
650.	-1474007.	-1265313.	101.682	---	---	---
700.	-1473201.	-1249290.	93.223	---	---	---
750.	-1472482.	-1233322.	85.896	---	---	---
(2 sigma)	1423.	739.	0.051	---	---	---
800.	-1471887.	-1217398.	79.488	---	---	---
850.	-1471458.	-1201507.	73.836	---	---	---
900.	-1471237.	-1185635.	68.812	---	---	---
950.	-1471270.	-1169769.	64.318	---	---	---
1000.	-1471604.	-1153893.	60.273	---	---	---
(2 sigma)	1469.	602.	0.031	---	---	---
1050.	-1473595.	-1137982.	56.611	---	---	---
1100.	-1473800.	-1121993.	53.279	---	---	---
1150.	-1473501.	-1106007.	50.236	---	---	---
1200.	-1474380.	-1090020.	57.447	---	---	---
1250.	-1472774.	-1074038.	44.882	---	---	---
(2 sigma)	1483.	484.	0.024	---	---	---
1300.	-1471064.	-1058121.	42.516	---	---	---
1350.	-1469233.	-1042273.	40.328	---	---	---
1400.	-1467264.	-1026496.	38.299	---	---	---
1450.	-1465137.	-1010791.	36.413	---	---	---
1500.	-1462834.	-995163.	34.655	---	---	---
(2 sigma)	2408.	713.	0.025	---	---	---
1550.	-1460335.	-979614.	33.013	---	---	---
1600.	-1457621.	-964150.	31.476	---	---	---
1650.	-1454670.	-948774.	30.036	---	---	---
1700.	-1503849.	-933005.	28.668	---	---	---
1750.	-1500572.	-916263.	27.349	---	---	---
(2 sigma)	5853.	1162.	0.035	---	---	---
1800.	-1497006.	-899618.	26.106	---	---	---
(2 sigma)	6897.	1328.	0.039	---	---	---

Table 102. Thermophysical values for magnetite, Fe_3O_4, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
200.	117.048	92.578	-13247.	-158.815	44.4806
250.	135.804	120.733	-6921.	-148.417	44.5025
(2 sigma)	0.196	0.504	8.	0.503	0.0149
273.15	143.597	133.106	-3685.	-146.598	44.5127
298.15	151.081	146.011	0.	-146.011	44.5236
(2 sigma)	0.174	0.503	0.	0.503	0.0159
300.	151.598	146.947	280.	-146.014	44.5244
350.	163.830	171.275	8179.	-147.907	44.5463
400.	173.572	193.808	16621.	-152.254	44.5683
450.	182.011	214.747	25514.	-158.048	44.5902
500.	190.153	234.344	34818.	-164.708	44.6121
(2 sigma)	0.646	0.522	67.	0.503	0.0615
550.	198.796	252.866	44538.	-171.888	44.6340
600.	208.567	270.572	54716.	-179.378	44.6559
650.	219.955	287.704	65422.	-187.055	44.6778
700.	233.348	304.481	76745.	-194.845	44.6998
750.	249.053	321.102	88795.	-202.708	44.7217
(2 sigma)	1.054	0.638	235.	0.510	0.1256
800.	267.320	337.744	101693.	-210.628	44.7436
848.50	337.	354.8	115400.	-218.8	44.7436
850.	300.9	355.3	115830.	-219.0	44.5420
900.	229.055	368.760	127968.	-226.573	44.5420
950.	217.256	380.801	139101.	-234.379	44.5420
1000.	210.378	391.753	149775.	-241.977	44.5420
(2 sigma)	1.254	2.788	2346.	0.650	---
1050.	206.725	401.918	160192.	-249.354	44.5420
1100.	205.108	411.492	170482.	-256.509	44.5420
1150.	204.704	420.597	180723.	-263.446	44.5420
1200.	204.944	429.313	190963.	-270.177	44.5420
1250.	205.442	437.689	201222.	-276.711	44.5420
(2 sigma)	5.143	2.924	2536.	1.012	---
1300.	205.948	445.756	211507.	-283.059	44.5420
1350.	206.306	453.536	221814.	-289.230	44.5420
1400.	206.429	461.042	232134.	-295.232	44.5420
1450.	206.282	468.284	242453.	-301.076	44.5420
1500.	205.867	475.271	252757.	-306.766	44.5420
(2 sigma)	5.169	3.314	3246.	1.321	---
1550.	205.208	482.011	263035.	-312.311	44.5420
1600.	204.353	488.514	273275.	-317.717	44.5420
1650.	203.358	494.787	283468.	-322.988	44.5420
1700.	202.289	500.842	293609.	-328.130	44.5420
1750.	201.220	506.690	303697.	-333.149	44.5420
(2 sigma)	3.702	3.631	3897.	1.593	---
1800.	200.223	512.345	313733.	-338.049	44.5420
(2 sigma)	3.685	3.663	3970.	1.643	---

Table 103. Thermochemical properties of magnetite, Fe_3O_4, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements. The properties relative to the oxides were not available. Refer to Section 1.5.5 for details.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-1116758.	-1048153.	273.749	---	---	---
250.	-1117732.	-1030843.	215.383	---	---	---
(2 sigma)	888.	828.	0.173	---	---	---
273.15	-1117613.	-1022800.	195.591	---	---	---
298.15	-1117262.	-1014137.	177.672	---	---	---
(2 sigma)	887.	818.	0.143	---	---	---
300.	-1117229.	-1013497.	176.465	---	---	---
350.	-1116096.	-996292.	148.688	---	---	---
400.	-1114659.	-979273.	127.880	---	---	---
450.	-1113030.	-962446.	111.718	---	---	---
500.	-1111226.	-945809.	98.808	---	---	---
(2 sigma)	897.	783.	0.082	---	---	---
550.	-1109216.	-929363.	88.263	---	---	---
600.	-1106948.	-913110.	79.493	---	---	---
650.	-1104355.	-897060.	72.089	---	---	---
700.	-1101366.	-881224.	65.758	---	---	---
750.	-1097905.	-865617.	60.287	---	---	---
(2 sigma)	944.	750.	0.052	---	---	---
800.	-1093896.	-850258.	55.516	---	---	---
848.50	-1089152.	-835993.	51.465	---	---	---
850.	-1089007.	-835509.	51.344	---	---	---
900.	-1086537.	-820324.	47.610	---	---	---
950.	-1085570.	-805566.	44.293	---	---	---
1000.	-1085640.	-790832.	41.309	---	---	---
(2 sigma)	2508.	841.	0.044	---	---	---
1050.	-1088591.	-776055.	38.607	---	---	---
1100.	-1089146.	-761157.	36.144	---	---	---
1150.	-1089164.	-746247.	33.896	---	---	---
1200.	-1091142.	-731310.	31.833	---	---	---
1250.	-1089587.	-716349.	29.935	---	---	---
(2 sigma)	2694.	1325.	0.055	---	---	---
1300.	-1088086.	-701449.	28.185	---	---	---
1350.	-1086642.	-686606.	26.566	---	---	---
1400.	-1085263.	-671816.	25.066	---	---	---
1450.	-1083960.	-657073.	23.670	---	---	---
1500.	-1082747.	-642373.	22.369	---	---	---
(2 sigma)	3380.	1985.	0.069	---	---	---
1550.	-1081634.	-627713.	21.154	---	---	---
1600.	-1080631.	-613087.	20.015	---	---	---
1650.	-1079746.	-598490.	18.947	---	---	---
1700.	-1081797.	-583864.	17.940	---	---	---
1750.	-1081682.	-569221.	16.990	---	---	---
(2 sigma)	4013.	2763.	0.082	---	---	---
1800.	-1081708.	-554580.	16.093	---	---	---
(2 sigma)	4084.	2929.	0.085	---	---	---

Table 104. Thermophysical values for the element hydrogen (H_2) at 1.01325 bars (1 atm). The sources of data are given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
200.	25.971	119.495	-2731.	-133.152	---
250.	28.057	125.552	-1372.	-131.041	---
(2 sigma)	---	---	---	---	---
273.15	28.513	128.058	-717.	-130.683	---
298.15	28.822	130.570	-0.	-130.570	---
(2 sigma)	---	---	---	---	---
300.	28.839	130.748	53.	-130.570	---
350.	29.127	135.219	1504.	-130.923	---
400.	29.221	139.116	2963.	-131.709	---
450.	29.244	142.559	4425.	-132.727	---
500.	29.250	145.641	5887.	-133.867	---
(2 sigma)	---	---	---	---	---
550.	29.263	148.429	7350.	-135.066	---
600.	29.293	150.977	8814.	-136.287	---
650.	29.345	153.323	10280.	-137.509	---
700.	29.417	155.500	11748.	-138.717	---
750.	29.511	157.533	13222.	-139.904	---
(2 sigma)	---	---	---	---	---
800.	29.623	159.441	14700.	-141.066	---
850.	29.751	161.241	16184.	-142.201	---
900.	29.895	162.945	17675.	-143.306	---
950.	30.052	164.566	19174.	-144.383	---
1000.	30.220	166.112	20681.	-145.431	---
(2 sigma)	---	---	---	---	---
1050.	30.397	167.590	22196.	-146.451	---
1100.	30.584	169.009	23720.	-147.445	---
1150.	30.777	170.372	25254.	-148.412	---
1200.	30.975	171.686	26798.	-149.354	---
1250.	31.179	172.955	28352.	-150.273	---
(2 sigma)	---	---	---	---	---
1300.	31.387	174.182	29916.	-151.169	---
1350.	31.597	175.370	31491.	-152.044	---
1400.	31.810	176.523	33076.	-152.898	---
1450.	32.024	177.643	34672.	-153.732	---
1500.	32.239	178.733	36278.	-154.547	---
(2 sigma)	---	---	---	---	---
1550.	32.455	179.793	37896.	-155.344	---
1600.	32.670	180.827	39524.	-156.125	---
1650.	32.885	181.836	41163.	-156.888	---
1700.	33.099	182.820	42812.	-157.637	---
1750.	33.311	183.783	44473.	-158.370	---
(2 sigma)	---	---	---	---	---
1800.	33.522	184.724	46143.	-159.089	---
(2 sigma)	---	---	---	---	---

Table 105. Thermochemical properties of the element hydrogen (H_2) at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	0.	0.	0.	---	---	---
250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
273.15	0.	0.	0.	---	---	---
298.15	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
300.	0.	0.	0.	---	---	---
350.	0.	0.	0.	---	---	---
400.	0.	0.	0.	---	---	---
450.	0.	0.	0.	---	---	---
500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
550.	0.	0.	0.	---	---	---
600.	0.	0.	0.	---	---	---
650.	0.	0.	0.	---	---	---
700.	0.	0.	0.	---	---	---
750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
800.	0.	0.	0.	---	---	---
850.	0.	0.	0.	---	---	---
900.	0.	0.	0.	---	---	---
950.	0.	0.	0.	---	---	---
1000.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1050.	0.	0.	0.	---	---	---
1100.	0.	0.	0.	---	---	---
1150.	0.	0.	0.	---	---	---
1200.	0.	0.	0.	---	---	---
1250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1300.	0.	0.	0.	---	---	---
1350.	0.	0.	0.	---	---	---
1400.	0.	0.	0.	---	---	---
1450.	0.	0.	0.	---	---	---
1500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1550.	0.	0.	0.	---	---	---
1600.	0.	0.	0.	---	---	---
1650.	0.	0.	0.	---	---	---
1700.	0.	0.	0.	---	---	---
1750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1800.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---

Table 106. Thermophysical values for stable phases with the composition H_2O at 1.01325 bars (1 atm). The tabulations are based on a fft of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C°_p J/(mol K)	S° J/(mol K)	$H^\circ_T - H^\circ_{298}$ J/mol	$[G^\circ_T - H^\circ_{298}]/T$ J/(mol K)	V° cm3/mol
		H_2O [liquid] = water			
273.15	75.884	63.307	-1888.	-70.218	18.0183
298.15	75.254	69.921	0.	-69.921	18.0683
(2 sigma)	---	---	---	---	---
300.	75.230	70.386	139.	-69.922	18.0772
350.	75.469	81.981	3900.	-70.837	18.5008
373.150	76.003	86.831	5653.	-71.681	18.7973
		H_2O [gas]			
373.150	34.048	196.318	46509.	-71.681	18.7973
400.	34.245	198.691	47425.	-80.127	---
450.	34.669	202.748	49148.	-93.530	---
500.	35.154	206.426	50893.	-104.639	---
(2 sigma)	---	---	---	---	---
550.	35.686	209.801	52664.	-114.048	---
600.	36.253	212.930	54463.	-122.159	---
650.	36.846	215.855	56290.	-129.255	---
700.	37.458	218.608	58147.	-135.540	---
750.	38.082	221.213	60036.	-141.165	---
(2 sigma)	---	---	---	---	---
800.	38.715	223.691	61956.	-146.247	---
850.	39.352	226.057	63907.	-150.872	---
900.	39.989	228.325	65891.	-155.113	---
950.	40.624	230.504	67906.	-159.024	---
1000.	41.254	232.604	69953.	-162.650	---
(2 sigma)	---	---	---	---	---
1050.	41.878	234.632	72032.	-166.030	---
1100.	42.494	236.594	74141.	-169.193	---
1150.	43.100	238.496	76281.	-172.165	---
1200.	43.695	240.343	78451.	-174.968	---
1250.	44.278	242.139	80650.	-177.619	---
(2 sigma)	---	---	---	---	---
1300.	44.848	243.887	82878.	-180.134	---
1350.	45.404	245.590	85135.	-182.527	---
1400.	45.945	247.251	87418.	-184.809	---
1450.	46.472	248.872	89729.	-186.990	---
1500.	46.982	250.456	92065.	-189.079	---
(2 sigma)	---	---	---	---	---
1550.	47.477	252.005	94427.	-191.084	---
1600.	47.954	253.520	96813.	-193.012	---
1650.	48.415	255.003	99222.	-194.868	---
1700.	48.858	256.455	101654.	-196.658	---
1750.	49.283	257.877	104108.	-198.387	---
(2 sigma)	---	---	---	---	---
1800.	49.689	259.271	106582.	-200.059	---
(2 sigma)	---	---	---	---	---

Table 107. Thermochemical properties of stable phases with the composition H_2O at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
		H_2O [liquid] = water				
273.15	-286613.	-241274.	46.139	0.0	0.0	0.0
298.15	-285808.	-237160.	41.549	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
300.	-285749.	-236858.	41.241	0.0	0.0	0.0
350.	-284178.	-228834.	34.152	0.0	0.0	0.0
373.150	-283447.	-225197.	31.524	0.0	0.0	0.0
		H_2O [gas]				
373.150	-242592.	-225197.	31.524	0.0	0.0	0.0
400.	-242865.	-223936.	29.243	0.0	0.0	0.0
450.	-243368.	-221539.	25.716	0.0	0.0	0.0
500.	-243861.	-219088.	22.888	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
550.	-244340.	-216587.	20.570	0.0	0.0	0.0
600.	-244804.	-214043.	18.634	0.0	0.0	0.0
650.	-245251.	-211462.	16.993	0.0	0.0	0.0
700.	-245681.	-208846.	15.584	0.0	0.0	0.0
750.	-246093.	-206201.	14.361	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
800.	-246488.	-203528.	13.289	0.0	0.0	0.0
850.	-246864.	-200832.	12.342	0.0	0.0	0.0
900.	-247224.	-198113.	11.498	0.0	0.0	0.0
950.	-247566.	-195375.	10.742	0.0	0.0	0.0
1000.	-247891.	-192620.	10.061	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1050.	-248200.	-189849.	9.444	0.0	0.0	0.0
1100.	-248492.	-187063.	8.883	0.0	0.0	0.0
1150.	-248769.	-184265.	8.370	0.0	0.0	0.0
1200.	-249031.	-181455.	7.899	0.0	0.0	0.0
1250.	-249278.	-178634.	7.465	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1300.	-249511.	-175803.	7.064	0.0	0.0	0.0
1350.	-249730.	-172964.	6.692	0.0	0.0	0.0
1400.	-249936.	-170117.	6.347	0.0	0.0	0.0
1450.	-250129.	-167263.	6.025	0.0	0.0	0.0
1500.	-250310.	-164403.	5.725	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1550.	-250480.	-161536.	5.444	0.0	0.0	0.0
1600.	-250638.	-158665.	5.180	0.0	0.0	0.0
1650.	-250786.	-155788.	4.932	0.0	0.0	0.0
1700.	-250923.	-152907.	4.698	0.0	0.0	0.0
1750.	-251051.	-150023.	4.478	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1800.	-251170.	-147134.	4.270	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0

Table 108. Thermophysical values for water, H_2O, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
273.15	75.884	63.307	-1888.	-70.218	18.0183
298.15	75.254	69.921	0.	-69.921	18.0683
(2 sigma)	---	---	---	---	---
300.	75.230	70.386	139.	-69.922	18.0772
350.	75.469	81.981	3900.	-70.837	18.5008
373.150	76.003	86.831	5653.	-71.681	18.7973
400.	76.849	92.140	7705.	-72.877	---
(2 sigma)	---	---	---	---	---

Table 109. Thermochemical properties of water, H_2O, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
273.15	-286613.	-241274.	46.139	0.0	0.0	0.0
298.15	-285808.	-237160.	41.549	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
300.	-285749.	-236858.	41.241	0.0	0.0	0.0
350.	-284178.	-228834.	34.152	0.0	0.0	0.0
373.150	-283447.	-225197.	31.524	0.0	0.0	0.0
400.	-282585.	-221036.	28.864	-39720.	2900.	-0.3787

Table 110. Thermophysical values for H_2O (ideal gas) at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
273.15	33.540	185.790	-840.	-188.864	---
298.15	33.632	188.731	0.	-188.731	---
(2 sigma)	---	---	---	---	---
300.	33.640	188.939	62.	-188.732	---
350.	33.897	194.143	1750.	-189.142	---
373.150	34.048	196.318	2537.	-189.520	---
400.	34.245	198.691	3453.	-190.057	---
450.	34.669	202.748	5176.	-191.246	---
500.	35.154	206.426	6921.	-192.583	---
(2 sigma)	---	---	---	---	---
550.	35.686	209.801	8692.	-193.997	---
600.	36.253	212.930	10491.	-195.446	---
650.	36.846	215.855	12318.	-196.904	---
700.	37.458	218.608	14175.	-198.357	---
750.	38.082	221.213	16064.	-199.795	---
(2 sigma)	---	---	---	---	---
800.	38.715	223.691	17984.	-201.211	---
850.	39.352	226.057	19935.	-202.604	---
900.	39.989	228.325	21919.	-203.970	---
950.	40.624	230.504	23934.	-205.310	---
1000.	41.254	232.604	25981.	-206.622	---
(2 sigma)	---	---	---	---	---
1050.	41.878	234.632	28060.	-207.908	---
1100.	42.494	236.594	30169.	-209.168	---
1150.	43.100	238.496	32309.	-210.402	---
1200.	43.695	240.343	34479.	-211.611	---
1250.	44.278	242.139	36678.	-212.796	---
(2 sigma)	---	---	---	---	---
1300.	44.848	243.887	38906.	-213.959	---
1350.	45.404	245.590	41163.	-215.099	---
1400.	45.945	247.251	43446.	-216.217	---
1450.	46.472	248.872	45757.	-217.316	---
1500.	46.982	250.456	48093.	-218.394	---
(2 sigma)	---	---	---	---	---
1550.	47.477	252.005	50455.	-219.453	---
1600.	47.954	253.520	52841.	-220.494	---
1650.	48.415	255.003	55250.	-221.518	---
1700.	48.858	256.455	57682.	-222.524	---
1750.	49.283	257.877	60136.	-223.514	---
(2 sigma)	---	---	---	---	---
1800.	49.689	259.271	62610.	-224.488	---
(2 sigma)	---	---	---	---	---

Table 111. Thermochemical properties of H_2O (ideal gas) at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
273.15	-241592.	-229710.	43.927	45021.	11564.	-2.211
298.15	-241836.	-228611.	40.052	43972.	8549.	-1.498
(2 sigma)	---	---	---	---	---	---
300.	-241854.	-228529.	39.790	43895.	8329.	-1.450
350.	-242357.	-226269.	33.769	41821.	2565.	-0.383
373.150	-242592.	-225197.	31.524	0.0	0.0	0.0
400.	-242865.	-223936.	29.243	0.0	0.0	0.0
450.	-243368.	-221539.	25.716	0.0	0.0	0.0
500.	-243861.	-219088.	22.888	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
550.	-244340.	-216587.	20.570	0.0	0.0	0.0
600.	-244804.	-214043.	18.634	0.0	0.0	0.0
650.	-245251.	-211462.	16.993	0.0	0.0	0.0
700.	-245681.	-208846.	15.584	0.0	0.0	0.0
750.	-246093.	-206201.	14.361	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
800.	-246488.	-203528.	13.289	0.0	0.0	0.0
850.	-246864.	-200832.	12.342	0.0	0.0	0.0
900.	-247224.	-198113.	11.498	0.0	0.0	0.0
950.	-247566.	-195375.	10.742	0.0	0.0	0.0
1000.	-247891.	-192620.	10.061	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1050.	-248200.	-189849.	9.444	0.0	0.0	0.0
1100.	-248492.	-187063.	8.883	0.0	0.0	0.0
1150.	-248769.	-184265.	8.370	0.0	0.0	0.0
1200.	-249031.	-181455.	7.899	0.0	0.0	0.0
1250.	-249278.	-178634.	7.465	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1300.	-249511.	-175803.	7.064	0.0	0.0	0.0
1350.	-249730.	-172964.	6.692	0.0	0.0	0.0
1400.	-249936.	-170117.	6.347	0.0	0.0	0.0
1450.	-250129.	-167263.	6.025	0.0	0.0	0.0
1500.	-250310.	-164403.	5.725	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1550.	-250480.	-161536.	5.444	0.0	0.0	0.0
1600.	-250638.	-158665.	5.180	0.0	0.0	0.0
1650.	-250786.	-155788.	4.932	0.0	0.0	0.0
1700.	-250923.	-152907.	4.698	0.0	0.0	0.0
1750.	-251051.	-150023.	4.478	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1800.	-251170.	-147134.	4.270	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0

Table 112. Thermophysical values for stable phases of the element magnesium (Mg) at 1.01325 bars (1 atm). The sources of data are given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
		magnesium (crystal)			
200.	22.761	23.170	-2347.	-34.908	---
250.	23.980	28.386	-1178.	-33.097	---
(2 sigma)	---	---	---	---	---
273.15	24.452	30.530	-617.	-32.789	---
298.15	24.905	32.692	-0.	-32.692	---
(2 sigma)	---	---	---	---	---
300.	24.937	32.846	46.	-32.692	---
350.	25.699	36.749	1313.	-32.999	---
400.	26.335	40.223	2614.	-33.688	---
450.	26.895	43.358	3945.	-34.592	---
500.	27.420	46.219	5303.	-35.613	---
(2 sigma)	---	---	---	---	---
550.	27.937	48.857	6687.	-36.699	---
600.	28.470	51.310	8097.	-37.815	---
650.	29.033	53.611	9534.	-38.943	---
700.	29.640	55.784	11001.	-40.069	---
750.	30.302	57.852	12499.	-41.186	---
(2 sigma)	---	---	---	---	---
800.	31.025	59.830	14032.	-42.290	---
850.	31.817	61.734	15603.	-43.378	---
900.	32.683	63.577	17215.	-44.449	---
922.	33.089	64.371	17939.	-44.915	---
		magnesium (liquid)			
922.	32.122	74.086	26895.	-44.915	---
950.	32.426	75.051	27799.	-45.789	---
1000.	32.970	76.728	29434.	-47.294	---
(2 sigma)	---	---	---	---	---
1050.	33.514	78.350	31096.	-48.735	---
1100.	34.058	79.922	32785.	-50.117	---
1150.	34.602	81.448	34502.	-51.446	---
1200.	35.146	82.932	36245.	-52.727	---
1250.	35.690	84.378	38016.	-53.964	---
(2 sigma)	---	---	---	---	---
1300.	36.234	85.788	39814.	-55.161	---
1350.	36.777	87.166	41640.	-56.321	---
1378.	37.082	87.924	42674.	-56.956	---
		magnesium (ideal monatomic gas)			
1378.	20.786	180.368	170062.	-56.956	---
1400.	20.786	180.697	170519.	-58.898	---
1450.	20.786	181.426	171558.	-63.110	---
1500.	20.786	182.131	172597.	-67.066	---
(2 sigma)	---	---	---	---	---
1550.	20.786	182.813	173637.	-70.789	---
1600.	20.786	183.473	174676.	-74.300	---
1650.	20.786	184.112	175715.	-77.618	---
1700.	20.786	184.733	176755.	-80.759	---
1750.	20.786	185.335	177794.	-83.739	---
(2 sigma)	---	---	---	---	---
1800.	20.786	185.921	178833.	-86.569	---
(2 sigma)	---	---	---	---	---

Table 113. Thermochemical properties of stable phases of the element magnesium (Mg) at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
		magnesium (crystal)				
200.	0.	0.	0.	---	---	---
250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
273.15	0.	0.	0.	---	---	---
298.15	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
300.	0.	0.	0.	---	---	---
350.	0.	0.	0.	---	---	---
400.	0.	0.	0.	---	---	---
450.	0.	0.	0.	---	---	---
500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
550.	0.	0.	0.	---	---	---
600.	0.	0.	0.	---	---	---
650.	0.	0.	0.	---	---	---
700.	0.	0.	0.	---	---	---
750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
800.	0.	0.	0.	---	---	---
850.	0.	0.	0.	---	---	---
900.	0.	0.	0.	---	---	---
922.	0.	0.	0.	---	---	---
		magnesium (liquid)				
922.	0.	0.	0.	---	---	---
950.	0.	0.	0.	---	---	---
1000.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1050.	0.	0.	0.	---	---	---
1100.	0.	0.	0.	---	---	---
1150.	0.	0.	0.	---	---	---
1200.	0.	0.	0.	---	---	---
1250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1300.	0.	0.	0.	---	---	---
1350.	0.	0.	0.	---	---	---
1378.	0.	0.	0.	---	---	---
		magnesium (ideal monatomic gas)				
1378.	0.	0.	0.	---	---	---
1400.	0.	0.	0.	---	---	---
1450.	0.	0.	0.	---	---	---
1500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1550.	0.	0.	0.	---	---	---
1600.	0.	0.	0.	---	---	---
1650.	0.	0.	0.	---	---	---
1700.	0.	0.	0.	---	---	---
1750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1800.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---

Table 114. Thermophysical values for magnesite, $MgCO_3$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
200.	57.411	38.410	-6618.	-71.498	27.9626
250.	67.903	52.385	-3476.	-66.291	27.9909
(2 sigma)	0.253	0.713	12.	0.712	0.0674
273.15	72.105	58.585	-1855.	-65.376	28.0040
298.15	76.233	65.081	0.	-65.081	28.0181
(2 sigma)	0.258	0.712	0.	0.712	0.0663
300.	76.523	65.553	141.	-65.082	28.0192
350.	83.648	77.901	4151.	-66.041	28.0474
400.	89.621	89.472	8487.	-68.254	28.0757
450.	94.706	100.329	13098.	-71.221	28.1040
500.	99.092	110.540	17946.	-74.648	28.1323
(2 sigma)	0.788	0.737	81.	0.713	0.0839
550.	102.923	120.168	22998.	-78.352	28.1606
600.	106.303	129.271	28231.	-82.220	28.1889
650.	109.312	137.901	33622.	-86.174	28.2172
700.	112.012	146.102	39157.	-90.164	28.2455
750.	114.453	153.915	44819.	-94.156	28.2738
(2 sigma)	1.690	0.968	384.	0.728	0.1328
800.	116.673	161.374	50598.	-98.126	28.3021
850.	118.702	168.509	56483.	-102.057	28.3304
900.	120.567	175.347	62466.	-105.940	28.3587
950.	122.288	181.912	68538.	-109.767	28.3870
1000.	123.883	188.226	74693.	-113.533	28.4153
(2 sigma)	2.347	1.415	886.	0.790	0.1906
1050.	125.366	194.307	80924.	-117.236	28.4436
1100.	126.750	200.171	87228.	-120.873	28.4719
1150.	128.045	205.834	93598.	-124.445	28.5001
1200.	129.260	211.309	100031.	-127.951	28.5284
1250.	130.403	216.610	106523.	-131.392	28.5567
(2 sigma)	2.831	1.928	1532.	0.914	0.2513
1300.	131.481	221.745	113070.	-134.768	28.5850
1350.	132.501	226.727	119670.	-138.082	28.6133
1400.	133.466	231.563	126319.	-141.335	28.6416
1450.	134.381	236.263	133015.	-144.528	28.6699
1500.	135.251	240.833	139756.	-147.662	28.6982
(2 sigma)	3.204	2.442	2285.	1.086	0.3132
1550.	136.080	245.282	146540.	-150.740	28.7265
1600.	136.870	249.615	153364.	-153.762	28.7548
1650.	137.624	253.838	160226.	-156.731	28.7831
1700.	138.346	257.957	167126.	-159.648	28.8114
1750.	139.036	261.978	174060.	-162.514	28.8397
(2 sigma)	3.500	2.936	3122.	1.286	0.3757
1800.	139.698	265.904	181029.	-165.332	28.8680
(2 sigma)	3.553	3.032	3297.	1.329	0.3882

Table 115. Thermochemical properties of magnesite, $MgCO_3$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-1112494.	-1056948.	276.046	-118309.	-83252.	21.743
250.	-1113039.	-1042989.	217.921	-118392.	-74476.	15.561
(2 sigma)	---	---	---	1786.	1735.	0.362
273.15	-1113161.	-1036497.	198.210	-118390.	-70409.	13.464
298.15	-1113225.	-1029477.	180.360	-118360.	-66019.	11.566
(2 sigma)	---	---	---	1785.	1727.	0.303
300.	-1113227.	-1028957.	179.157	-118357.	-65694.	11.438
350.	-1113176.	-1014913.	151.467	-118212.	-56927.	8.496
400.	-1112953.	-1000889.	130.703	-117968.	-48188.	6.293
450.	-1112599.	-986901.	114.556	-117634.	-39484.	4.583
500.	-1112141.	-972959.	101.644	-117222.	-30823.	3.220
(2 sigma)	---	---	---	1796.	1700.	0.178
550.	-1111599.	-959066.	91.084	-116739.	-22205.	2.109
600.	-1110991.	-945226.	82.289	-116192.	-13635.	1.187
650.	-1110328.	-931438.	74.851	-115587.	-5113.	0.411
700.	-1109623.	-917704.	68.480	-114928.	3361.	-0.251
750.	-1108885.	-904021.	62.962	-114221.	11786.	-0.821
(2 sigma)	---	---	---	1867.	1677.	0.117
800.	-1108123.	-890388.	58.136	-113468.	20162.	-1.316
850.	-1107345.	-876803.	53.882	-112673.	28489.	-1.751
900.	-1106559.	-863265.	50.103	-111840.	36769.	-2.134
950.	-1114699.	-849498.	46.709	-110970.	45002.	-2.474
1000.	-1113847.	-835562.	43.645	-110067.	53188.	-2.778
(2 sigma)	---	---	---	2075.	1684.	0.088
1050.	-1112981.	-821669.	40.876	-109131.	61327.	-3.051
1100.	-1112103.	-807818.	38.360	-108166.	69422.	-3.297
1150.	-1111216.	-794007.	36.065	-107173.	77472.	-3.519
1200.	-1110321.	-780234.	33.963	-106153.	85478.	-3.721
1250.	-1109419.	-766499.	32.030	-105108.	93442.	-3.905
(2 sigma)	---	---	---	2470.	1779.	0.074
1300.	-1108512.	-752800.	30.248	-104039.	101363.	-4.073
1350.	-1107600.	-739136.	28.599	-102948.	109242.	-4.227
1400.	-1232139.	-721902.	26.934	-101837.	117081.	-4.368
1450.	-1230381.	-703710.	25.350	-100705.	124879.	-4.499
1500.	-1228594.	-685579.	23.874	-99554.	132638.	-4.619
(2 sigma)	---	---	---	3039.	2027.	0.071
1550.	-1226779.	-667509.	22.495	-98386.	140359.	-4.730
1600.	-1224936.	-649497.	21.204	-97200.	148041.	-4.833
1650.	-1223066.	-631543.	19.993	-95999.	155687.	-4.929
1700.	-1221169.	-613647.	18.855	-94783.	163295.	-5.017
1750.	-1219245.	-595807.	17.784	-93552.	170868.	-5.100
(2 sigma)	---	---	---	3749.	2465.	0.074
1800.	-1217295.	-578022.	16.774	-92308.	178405.	-5.177
(2 sigma)	---	---	---	3904.	2575.	0.075

Table 116. Thermophysical values for periclase, MgO, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T	C_p°	S°	$H_T^\circ - H_{298}^\circ$	$[G_T^\circ - H_{298}^\circ]/T$	V°
K	J/(mol K)	J/(mol K)	J/mol	J/(mol K)	cm3/mol
200.	26.590	14.005	-3217.	-30.089	11.2031
250.	33.261	20.719	-1706.	-27.544	11.2240
(2 sigma)	---	---	---	---	0.0090
273.15	35.424	23.762	-910.	-27.095	11.2336
298.15	37.344	26.950	0.	-26.950	11.2441
(2 sigma)	---	---	---	---	0.0083
300.	37.472	27.181	69.	-26.950	11.2449
350.	40.380	33.188	2020.	-27.418	11.2657
400.	42.514	38.726	4094.	-28.490	11.2866
450.	44.151	43.832	6263.	-29.915	11.3075
500.	45.446	48.554	8504.	-31.546	11.3284
(2 sigma)	---	---	---	---	0.0064
550.	46.499	52.936	10803.	-33.294	11.3493
600.	47.373	57.021	13151.	-35.103	11.3702
650.	48.111	60.842	15538.	-36.937	11.3911
700.	48.743	64.432	17960.	-38.774	11.4120
750.	49.292	67.814	20411.	-40.599	11.4329
(2 sigma)	---	---	---	---	0.0074
800.	49.774	71.011	22888.	-42.400	11.4538
850.	50.203	74.041	25388.	-44.173	11.4747
900.	50.588	76.922	27908.	-45.913	11.4956
950.	50.938	79.666	30446.	-47.618	11.5165
1000.	51.258	82.288	33001.	-49.286	11.5374
(2 sigma)	---	---	---	---	0.0110
1050.	51.554	84.796	35571.	-50.918	11.5583
1100.	51.831	87.200	38156.	-52.513	11.5792
1150.	52.090	89.510	40754.	-54.072	11.6001
1200.	52.337	91.732	43365.	-55.595	11.6209
1250.	52.572	93.874	45988.	-57.083	11.6418
(2 sigma)	---	---	---	---	0.0154
1300.	52.799	95.940	48622.	-58.538	11.6627
1350.	53.019	97.937	51268.	-59.961	11.6836
1400.	53.234	99.869	53924.	-61.352	11.7045
1450.	53.445	101.741	56591.	-62.712	11.7254
1500.	53.653	103.556	59268.	-64.044	11.7463
(2 sigma)	---	---	---	---	0.0202
1550.	53.860	105.319	61956.	-65.347	11.7672
1600.	54.066	107.032	64654.	-66.623	11.7881
1650.	54.273	108.699	67363.	-67.873	11.8090
1700.	54.480	110.322	70082.	-69.098	11.8299
1750.	54.689	111.904	72811.	-70.298	11.8508
(2 sigma)	---	---	---	---	0.0252
1800.	54.900	113.448	75551.	-71.475	11.8717
(2 sigma)	---	---	---	---	0.0262

Table 117. Thermochemical properties of periclase, MgO, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-600677.	-579505.	151.351	0.0	0.0	0.0
250.	-601064.	-574161.	119.964	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
273.15	-601166.	-571665.	109.320	0.0	0.0	0.0
298.15	-601239.	-568961.	99.680	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
300.	-601243.	-568761.	99.030	0.0	0.0	0.0
350.	-601299.	-563342.	84.074	0.0	0.0	0.0
400.	-601277.	-557920.	72.857	0.0	0.0	0.0
450.	-601204.	-552504.	64.133	0.0	0.0	0.0
500.	-601097.	-547099.	57.155	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
550.	-600969.	-541705.	51.447	0.0	0.0	0.0
600.	-600830.	-536323.	46.691	0.0	0.0	0.0
650.	-600688.	-530954.	42.668	0.0	0.0	0.0
700.	-600552.	-525594.	39.220	0.0	0.0	0.0
750.	-600426.	-520245.	36.233	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
800.	-600318.	-514903.	33.620	0.0	0.0	0.0
850.	-600234.	-509567.	31.314	0.0	0.0	0.0
900.	-600178.	-504236.	29.265	0.0	0.0	0.0
950.	-609082.	-498635.	27.417	0.0	0.0	0.0
1000.	-609027.	-492823.	25.742	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1050.	-608990.	-487014.	24.228	0.0	0.0	0.0
1100.	-608973.	-481206.	22.851	0.0	0.0	0.0
1150.	-608974.	-475399.	21.593	0.0	0.0	0.0
1200.	-608995.	-469591.	20.441	0.0	0.0	0.0
1250.	-609035.	-463782.	19.380	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1300.	-609096.	-457970.	18.401	0.0	0.0	0.0
1350.	-609177.	-452156.	17.495	0.0	0.0	0.0
1400.	-734731.	-442735.	16.519	0.0	0.0	0.0
1450.	-734011.	-432319.	15.574	0.0	0.0	0.0
1500.	-733284.	-421928.	14.693	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1550.	-732549.	-411562.	13.870	0.0	0.0	0.0
1600.	-731806.	-401219.	13.098	0.0	0.0	0.0
1650.	-731055.	-390900.	12.375	0.0	0.0	0.0
1700.	-730295.	-380604.	11.695	0.0	0.0	0.0
1750.	-729527.	-370330.	11.054	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1800.	-728749.	-360078.	10.449	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0

Table 118. Thermophysical values for brucite, $Mg(OH)_2$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
200.	55.856	36.369	-6661.	-69.673	24.5785
250.	68.611	50.285	-3531.	-64.408	24.6052
(2 sigma)	0.152	0.662	6.	0.662	0.3555
273.15	73.261	56.568	-1888.	-63.479	24.6176
298.15	77.641	63.178	0.	-63.178	24.6309
(2 sigma)	0.099	0.662	0.	0.662	0.3552
300.	77.942	63.659	144.	-63.179	24.6319
350.	85.123	76.235	4228.	-64.156	24.6586
400.	90.849	87.989	8632.	-66.409	24.6853
450.	95.538	98.969	13295.	-69.423	24.7120
500.	99.455	109.244	18173.	-72.897	24.7387
(2 sigma)	0.092	0.662	14.	0.662	0.3587
550.	102.780	118.883	23231.	-76.644	24.7654
600.	105.639	127.951	28443.	-80.546	24.7921
650.	108.125	136.507	33789.	-84.524	24.8188
700.	110.304	144.602	39251.	-88.529	24.8455
750.	112.228	152.279	44815.	-92.526	24.8722
(2 sigma)	0.164	0.665	39.	0.662	0.3729
800.	113.939	159.578	50470.	-96.490	24.8989
850.	115.468	166.532	56206.	-100.407	24.9256
900.	116.841	173.171	62014.	-104.267	24.9523
950.	118.078	179.522	67888.	-108.062	24.9790
1000.	119.197	185.608	73820.	-111.788	25.0057
(2 sigma)	0.281	0.672	86.	0.663	0.3969
1050.	120.212	191.448	79806.	-115.443	25.0324
1100.	121.135	197.062	85840.	-119.026	25.0591
1150.	121.975	202.466	91918.	-122.537	25.0858
1200.	122.743	207.673	98036.	-125.977	25.1125
1250.	123.445	212.698	104191.	-129.346	25.1391
(2 sigma)	0.430	0.686	166.	0.664	0.4290

Table 119. Thermochemical properties of brucite, $Mg(OH)_2$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	-924028.	-864090.	225.677	---	---	---
250.	-924881.	-848996.	177.388	---	---	---
(2 sigma)	---	---	---	---	---	---
273.15	-925129.	-841958.	161.008	-37350.	-29019.	5.549
298.15	-925307.	-834337.	146.172	-38261.	-28215.	4.943
(2 sigma)	---	---	---	1258.	1175.	0.206
300.	-925317.	-833772.	145.173	-38325.	-28153.	4.902
350.	-925431.	-818502.	122.155	-39953.	-26326.	3.929
400.	-925290.	-803233.	104.891	-81149.	-21377.	2.792
450.	-924948.	-787995.	91.468	-80376.	-13951.	1.619
500.	-924443.	-772803.	80.734	-79485.	-6617.	0.691
(2 sigma)	---	---	---	1258.	1135.	0.119
550.	-923806.	-757669.	71.957	-78497.	622.	-0.059
600.	-923065.	-742598.	64.649	-77431.	7769.	-0.676
650.	-922240.	-727592.	58.470	-76300.	14823.	-1.191
700.	-921351.	-712652.	53.179	-75118.	21789.	-1.626
750.	-920413.	-697777.	48.598	-73893.	28668.	-1.997
(2 sigma)	---	---	---	1259.	1106.	0.077
800.	-919441.	-682967.	44.593	-72635.	35465.	-2.316
850.	-918448.	-668217.	41.064	-71350.	42182.	-2.592
900.	-917447.	-653527.	37.930	-70045.	48822.	-2.834
950.	-925373.	-638620.	35.114	-68726.	55390.	-3.046
1000.	-924313.	-623555.	32.571	-67395.	61888.	-3.233
(2 sigma)	---	---	---	1262.	1102.	0.058
1050.	-923248.	-608544.	30.273	-66058.	68319.	-3.399
1100.	-922183.	-593583.	28.187	-64718.	74687.	-3.547
1150.	-921121.	-578670.	26.284	-63378.	80994.	-3.679
1200.	-920066.	-563804.	24.542	-62041.	87242.	-3.798
1250.	-919021.	-548981.	22.941	-60708.	93435.	-3.904
(2 sigma)	---	---	---	1271.	1123.	0.047

Table 120. Thermophysical values for Mg pyroxene, $MgSiO_3$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T	C_p°	S°	$H_T^\circ - H_{298}^\circ$	$[G_T^\circ - H_{298}^\circ]/T$	V°
K	J/(mol K)	J/(mol K)	J/mol	J/(mol K)	cm3/mol
		clinoenstatite			
200.	58.831	39.463	-7030.	-74.611	31.1757
250.	72.520	54.170	-3721.	-69.056	31.2256
(2 sigma)	0.117	1.811	6.	1.810	0.0282
273.15	77.237	60.804	-1987.	-68.077	31.2487
298.15	81.569	67.760	0.	-67.760	31.2736
(2 sigma)	0.145	1.810	0.	1.810	0.0238
300.	81.864	68.266	151.	-67.762	31.2755
350.	88.756	81.427	4425.	-68.785	31.3254
400.	94.112	93.642	9001.	-71.139	31.3752
450.	98.429	104.985	13819.	-74.277	31.4251
500.	102.007	115.546	18832.	-77.882	31.4750
(2 sigma)	0.183	1.810	36.	1.810	0.0466
550.	105.036	125.414	24010.	-81.759	31.5248
600.	107.644	134.668	29329.	-85.787	31.5747
650.	109.922	143.376	34769.	-89.885	31.6246
700.	111.934	151.597	40316.	-94.002	31.6744
750.	113.728	159.382	45959.	-98.104	31.7243
(2 sigma)	0.159	1.812	75.	1.810	0.0997
800.	115.341	166.774	51686.	-102.167	31.7742
850.	116.802	173.811	57490.	-106.176	31.8241
900.	118.134	180.526	63364.	-110.121	31.8739
950.	119.354	186.946	69302.	-113.997	31.9238
968.500	119.780	189.252	71514.	-115.412	31.9423
		enstatite			
968.500	125.855	192.652	74806.	-115.512	31.9376
1000.	126.493	196.690	78781.	-117.909	31.9692
(2 sigma)	0.099	0.342	1820.	1.795	0.1073
1050.	127.405	202.884	85129.	-121.809	32.0197
1100.	128.207	208.830	91519.	-125.631	32.0704
1150.	128.913	214.545	97948.	-129.373	32.1214
1200.	129.530	220.045	104409.	-133.037	32.1727
1250.	130.069	225.344	110899.	-136.624	32.2241
(2 sigma)	0.189	0.345	1821.	1.439	0.2139
1257.400	130.143	226.112	111862.	-137.148	32.2317
		protoenstatite			
1257.400	120.006	229.007	115504.	-137.147	33.2299
1300.	120.634	233.016	120630.	-140.224	33.2695
1350.	121.332	237.582	126679.	-143.745	33.3159
1400.	121.992	242.007	132763.	-147.176	33.3624
1450.	122.619	246.298	138878.	-150.520	33.4089
1500.	123.213	250.466	145024.	-153.783	33.4554
(2 sigma)	3.716	1.272	2435.	1.220	0.1137
1550.	123.778	254.515	151199.	-156.967	33.5019
1600.	124.317	258.453	157401.	-160.077	33.5484
1650.	124.831	262.287	163630.	-163.117	33.5949
1700.	125.322	266.021	169884.	-166.089	33.6414
1750.	125.792	269.660	176162.	-168.996	33.6879
(2 sigma)	4.048	1.368	2608.	1.087	0.1479
1800.	126.243	273.210	182463.	-171.842	33.7343
(2 sigma)	4.108	1.415	2687.	1.068	0.1550

Table 121. Thermochemical properties of My pyroxene, $MgSiO_3$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
			clinoenstatite			
200.	-1543460.	-1486369.	388.200	-32903.	-32789.	8.564
250.	-1544355.	-1471983.	307.554	-32917.	-32759.	6.845
(2 sigma)	---	---	---	4087.	4021.	0.840
273.15	-1544626.	-1465269.	280.204	-32924.	-32744.	6.262
298.15	-1544844.	-1457995.	255.435	-32935.	-32727.	5.734
(2 sigma)	---	---	---	4087.	4014.	0.703
300.	-1544857.	-1457456.	253.766	-32936.	-32726.	5.698
350.	-1545103.	-1442867.	215.336	-32973.	-32689.	4.879
400.	-1545168.	-1428256.	186.511	-33036.	-32644.	4.263
450.	-1545100.	-1413645.	164.091	-33128.	-32590.	3.783
500.	-1544932.	-1399047.	146.157	-33255.	-32524.	3.398
(2 sigma)	---	---	---	4087.	4005.	0.418
550.	-1544687.	-1384470.	131.486	-33417.	-32443.	3.081
600.	-1544383.	-1369917.	119.262	-33617.	-32346.	2.816
650.	-1544035.	-1355392.	108.921	-33857.	-32230.	2.590
700.	-1543657.	-1340896.	100.059	-34137.	-32095.	2.395
750.	-1543258.	-1326426.	92.380	-34460.	-31938.	2.224
(2 sigma)	---	---	---	4087.	4040.	0.281
800.	-1542848.	-1311984.	85.664	-34826.	-31758.	2.074
850.	-1542436.	-1297568.	79.739	-35947.	-31549.	1.939
900.	-1542030.	-1283176.	74.474	-35978.	-31289.	1.816
950.	-1550564.	-1268534.	69.749	-35989.	-31029.	1.706
968.500	-1550399.	-1263044.	68.120	-35988.	-30932.	1.668
			enstatite			
968.500	-1547107.	-1263044.	68.120	-32696.	-30932.	1.668
1000.	-1546637.	-1253812.	65.492	-32500.	-30878.	1.613
(2 sigma)	---	---	---	4108.	4099.	0.214
1050.	-1545896.	-1239189.	61.646	-32183.	-30804.	1.532
1100.	-1545166.	-1224601.	58.151	-31862.	-30746.	1.460
1150.	-1544450.	-1210046.	54.962	-31542.	-30703.	1.395
1200.	-1543750.	-1195522.	52.040	-31227.	-30673.	1.335
1250.	-1543070.	-1181027.	49.352	-30920.	-30656.	1.281
(2 sigma)	---	---	---	4108.	4101.	0.171
1257.400	-1542972.	-1178884.	48.973	-30875.	-30655.	1.273
			protoenstatite			
1257.400	-1539329.	-1178884.	48.973	-27233.	-30655.	1.273
1300.	-1539197.	-1166673.	46.877	-27409.	-30767.	1.236
1350.	-1539051.	-1152348.	44.587	-27616.	-30892.	1.195
1400.	-1664368.	-1134424.	42.326	-27825.	-31009.	1.157
1450.	-1663403.	-1115514.	40.185	-28037.	-31119.	1.121
1500.	-1662422.	-1096638.	38.188	-28255.	-31222.	1.087
(2 sigma)	---	---	---	4409.	4117.	0.143
1550.	-1661425.	-1077795.	36.321	-28479.	-31317.	1.055
1600.	-1660413.	-1058985.	34.572	-28711.	-31405.	1.025
1650.	-1659386.	-1040206.	32.930	-28952.	-31486.	0.997
1700.	-1708854.	-1021008.	31.372	-29203.	-31559.	0.970
1750.	-1707655.	-1000795.	29.872	-29466.	-31624.	0.944
(2 sigma)	---	---	---	4507.	4151.	0.124
1800.	-1706437.	-980616.	28.457	-29742.	-31682.	0.919
(2 sigma)	---	---	---	4554.	4160.	0.121

Table 122. Thermophysical values for clinoenstatite, $MgSiO_3$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
200.	58.831	39.463	-7030.	-74.611	31.1757
250.	72.520	54.170	-3721.	-69.056	31.2256
(2 sigma)	0.117	1.811	6.	1.810	0.0282
273.15	77.237	60.804	-1987.	-68.077	31.2487
298.15	81.569	67.760	0.	-67.760	31.2736
(2 sigma)	0.145	1.810	0.	1.810	0.0238
300.	81.864	68.266	151.	-67.762	31.2755
350.	88.756	81.427	4425.	-68.785	31.3254
400.	94.112	93.642	9001.	-71.139	31.3752
450.	98.429	104.985	13819.	-74.277	31.4251
500.	102.007	115.546	18832.	-77.882	31.4750
(2 sigma)	0.183	1.810	36.	1.810	0.0466
550.	105.036	125.414	24010.	-81.759	31.5248
600.	107.644	134.668	29329.	-85.787	31.5747
650.	109.922	143.376	34769.	-89.885	31.6246
700.	111.934	151.597	40316.	-94.002	31.6744
750.	113.728	159.382	45959.	-98.104	31.7243
(2 sigma)	0.159	1.812	75.	1.810	0.0997
800.	115.341	166.774	51686.	-102.167	31.7742
850.	116.802	173.811	57490.	-106.176	31.8241
900.	118.134	180.526	63364.	-110.121	31.8739
950.	119.354	186.946	69302.	-113.997	31.9238
968.500	119.780	189.252	71514.	-115.412	31.9423
1000.	120.478	193.097	75298.	-117.799	31.9737
(2 sigma)	0.177	1.814	107.	1.810	0.1552
1050.	121.517	199.001	81348.	-121.526	32.0235
1100.	122.482	204.676	87448.	-125.178	32.0734
1150.	123.381	210.141	93595.	-128.754	32.1233
1200.	124.222	215.410	99786.	-132.255	32.1732
1250.	125.010	220.497	106017.	-135.684	32.2230
(2 sigma)	0.214	1.816	141.	1.810	0.2112
1300.	125.751	225.415	112286.	-139.041	32.2729
1350.	126.449	230.174	118591.	-142.328	32.3228
1400.	127.108	234.784	124930.	-145.549	32.3726
1450.	127.733	239.256	131301.	-148.703	32.4225
1500.	128.325	243.596	137703.	-151.794	32.4724
(2 sigma)	0.251	1.819	184.	1.811	0.2674
1550.	128.887	247.813	144133.	-154.824	32.5222
1600.	129.423	251.914	150591.	-157.794	32.5721
1650.	129.933	255.904	157075.	-160.707	32.6220
1700.	130.421	259.790	163584.	-163.564	32.6719
1750.	130.887	263.578	170117.	-166.368	32.7217
(2 sigma)	0.285	1.822	238.	1.812	0.3237
1800.	131.333	267.271	176672.	-169.120	32.7716
(2 sigma)	0.291	1.822	250.	1.812	0.3350

Table 123. Thermochemical properties of clinoenstatite, $MgSiO_3$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-1543460.	-1486369.	388.200	-32903.	-32789.	8.564
250.	-1544355.	-1471983.	307.554	-32917.	-32759.	6.845
(2 sigma)	---	---	---	4087.	4021.	0.840
273.15	-1544626.	-1465269.	280.204	-32924.	-32744.	6.262
298.15	-1544844.	-1457995.	255.435	-32935.	-32727.	5.734
(2 sigma)	---	---	---	4087.	4014.	0.703
300.	-1544857.	-1457456.	253.766	-32936.	-32726.	5.698
350.	-1545103.	-1442867.	215.336	-32973.	-32689.	4.879
400.	-1545168.	-1428256.	186.511	-33036.	-32644.	4.263
450.	-1545100.	-1413645.	164.091	-33128.	-32590.	3.783
500.	-1544932.	-1399047.	146.157	-33255.	-32524.	3.398
(2 sigma)	---	---	---	4087.	4005.	0.418
550.	-1544687.	-1384470.	131.486	-33417.	-32443.	3.081
600.	-1544383.	-1369917.	119.262	-33617.	-32346.	2.816
650.	-1544035.	-1355392.	108.921	-33857.	-32230.	2.590
700.	-1543657.	-1340896.	100.059	-34137.	-32095.	2.395
750.	-1543258.	-1326426.	92.380	-34460.	-31938.	2.224
(2 sigma)	---	---	---	4087.	4040.	0.281
800.	-1542848.	-1311984.	85.664	-34826.	-31758.	2.074
850.	-1542436.	-1297568.	79.739	-35947.	-31549.	1.939
900.	-1542030.	-1283176.	74.474	-35978.	-31289.	1.816
950.	-1550564.	-1268534.	69.749	-35989.	-31029.	1.706
968.500	-1550399.	-1263044.	68.120	-35988.	-30932.	1.668
1000.	-1550120.	-1253702.	65.487	-35983.	-30768.	1.607
(2 sigma)	---	---	---	4087.	4125.	0.215
1050.	-1549677.	-1238892.	61.631	-35963.	-30507.	1.518
1100.	-1549237.	-1224103.	58.128	-35933.	-30248.	1.436
1150.	-1548802.	-1209334.	54.930	-35894.	-29991.	1.362
1200.	-1548374.	-1194584.	51.999	-35850.	-29735.	1.294
1250.	-1547953.	-1179851.	49.303	-35803.	-29481.	1.232
(2 sigma)	---	---	---	4088.	4258.	0.178
1300.	-1547541.	-1165135.	46.816	-35753.	-29229.	1.174
1350.	-1547139.	-1150435.	44.513	-35704.	-28979.	1.121
1400.	-1672201.	-1132145.	42.241	-35658.	-28731.	1.072
1450.	-1670980.	-1112879.	40.090	-35614.	-28484.	1.026
1500.	-1669743.	-1093655.	38.084	-35576.	-28239.	0.983
(2 sigma)	---	---	---	4089.	4433.	0.154
1550.	-1668491.	-1074473.	36.209	-35545.	-27995.	0.943
1600.	-1667223.	-1055331.	34.453	-35521.	-27752.	0.906
1650.	-1665941.	-1036229.	32.804	-35507.	-27509.	0.871
1700.	-1715154.	-1016717.	31.240	-35504.	-27267.	0.838
1750.	-1713700.	-996196.	29.735	-35512.	-27025.	0.807
(2 sigma)	---	---	---	4091.	4646.	0.139
1800.	-1712228.	-975716.	28.315	-35532.	-26782.	0.777
(2 sigma)	---	---	---	4092.	4693.	0.136

Table 124. Thermophysical values for enstatite, $MgSiO_3$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
200.	58.925	37.989	-7034.	-73.158	31.2970
250.	72.421	52.665	-3733.	-67.596	31.3221
(2 sigma)	0.067	0.338	3.	0.337	0.0658
273.15	77.440	59.303	-1997.	-66.613	31.3351
298.15	82.203	66.294	0.	-66.294	31.3501
(2 sigma)	0.065	0.337	0.	0.337	0.0355
300.	82.532	66.804	152.	-66.296	31.3513
350.	90.396	80.141	4483.	-67.331	31.3841
400.	96.688	92.637	9166.	-69.722	31.4198
450.	101.832	104.332	14133.	-72.925	31.4582
500.	106.110	115.289	19335.	-76.619	31.4986
(2 sigma)	0.060	0.339	11.	0.337	0.0895
550.	109.714	125.576	24733.	-80.607	31.5410
600.	112.785	135.257	30297.	-84.762	31.5848
650.	115.423	144.392	36004.	-89.001	31.6300
700.	117.705	153.031	41834.	-93.269	31.6762
750.	119.690	161.221	47770.	-97.528	31.7234
(2 sigma)	0.072	0.341	24.	0.338	0.0858
800.	121.425	169.002	53798.	-101.754	31.7714
850.	122.945	176.410	59909.	-105.930	31.8201
900.	124.281	183.476	66090.	-110.043	31.8694
950.	125.457	190.228	72334.	-114.087	31.9191
968.500	125.855	192.652	74659.	-115.565	31.9376
1000.	126.493	196.690	78633.	-118.057	31.9692
(2 sigma)	0.099	0.342	37.	0.338	0.1073
1050.	127.405	202.884	84981.	-121.950	32.0197
1100.	128.207	208.830	91372.	-125.765	32.0704
1150.	128.913	214.545	97800.	-129.501	32.1214
1200.	129.530	220.045	104262.	-133.160	32.1727
1250.	130.069	225.344	110752.	-136.742	32.2241
(2 sigma)	0.189	0.345	58.	0.339	0.2139
1257.400	130.143	226.112	111715.	-137.266	32.2317
1300.	130.537	230.454	117267.	-140.249	32.2756
1350.	130.940	235.389	123805.	-143.681	32.3273
1400.	131.285	240.157	130360.	-147.042	32.3791
1450.	131.576	244.769	136932.	-150.333	32.4309
1500.	131.818	249.234	143517.	-153.556	32.4829
(2 sigma)	0.320	0.351	108.	0.339	0.3497
1550.	132.014	253.560	150113.	-156.712	32.5349
1600.	132.169	257.753	156718.	-159.805	32.5870
1650.	132.285	261.822	163329.	-162.835	32.6391
1700.	132.365	265.773	169946.	-165.805	32.6912
1750.	132.413	269.610	176565.	-168.716	32.7434
(2 sigma)	0.472	0.367	198.	0.340	0.4953
1800.	132.429	273.341	183187.	-171.571	32.7956
(2 sigma)	0.504	0.372	221.	0.341	0.5250

Table 125. Thermochemical properties of enstatite, $MgSiO_3$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-1543316.	-1485931.	388.085	-32759.	-32351.	8.449
250.	-1544219.	-1471471.	307.447	-32781.	-32247.	6.738
(2 sigma)	---	---	---	4108.	4103.	0.857
273.15	-1544489.	-1464721.	280.099	-32787.	-32197.	6.157
298.15	-1544696.	-1457411.	255.332	-32788.	-32143.	5.631
(2 sigma)	---	---	---	4108.	4102.	0.719
300.	-1544708.	-1456869.	253.663	-32788.	-32139.	5.596
350.	-1544897.	-1442211.	215.238	-32767.	-32032.	4.781
400.	-1544856.	-1427542.	186.418	-32724.	-31930.	4.170
450.	-1544639.	-1412889.	164.004	-32666.	-31834.	3.695
500.	-1544282.	-1398268.	146.076	-32605.	-31745.	3.316
(2 sigma)	---	---	---	4108.	4100.	0.428
550.	-1543817.	-1383689.	131.412	-32547.	-31662.	3.007
600.	-1543267.	-1369155.	119.195	-32501.	-31584.	2.750
650.	-1542653.	-1354670.	108.863	-32474.	-31508.	2.532
700.	-1541992.	-1340235.	100.009	-32473.	-31434.	2.346
750.	-1541299.	-1325847.	92.340	-32502.	-31359.	2.184
(2 sigma)	---	---	---	4108.	4098.	0.285
800.	-1540588.	-1311507.	85.633	-32566.	-31281.	2.042
850.	-1539870.	-1297212.	79.717	-33382.	-31193.	1.917
900.	-1539157.	-1282958.	74.461	-33105.	-31072.	1.803
950.	-1547384.	-1268473.	69.745	-32809.	-30967.	1.703
968.500	-1547107.	-1263044.	68.120	-32696.	-30932.	1.668
1000.	-1546637.	-1253812.	65.492	-32500.	-30878.	1.613
(2 sigma)	---	---	---	4108.	4099.	0.214
1050.	-1545896.	-1239189.	61.646	-32183.	-30804.	1.532
1100.	-1545166.	-1224601.	58.151	-31862.	-30746.	1.460
1150.	-1544450.	-1210046.	54.962	-31542.	-30703.	1.395
1200.	-1543750.	-1195522.	52.040	-31227.	-30673.	1.335
1250.	-1543070.	-1181027.	49.352	-30920.	-30656.	1.281
(2 sigma)	---	---	---	4108.	4101.	0.171
1257.400	-1542972.	-1178884.	48.973	-30875.	-30655.	1.273
1300.	-1542412.	-1166558.	46.873	-30624.	-30652.	1.232
1350.	-1541778.	-1152114.	44.578	-30343.	-30658.	1.186
1400.	-1666623.	-1134089.	42.313	-30080.	-30675.	1.144
1450.	-1665201.	-1115095.	40.170	-29836.	-30700.	1.106
1500.	-1663781.	-1096150.	38.171	-29614.	-30734.	1.070
(2 sigma)	---	---	---	4109.	4105.	0.143
1550.	-1662363.	-1077253.	36.303	-29417.	-30775.	1.037
1600.	-1660949.	-1058401.	34.553	-29247.	-30821.	1.006
1650.	-1659540.	-1039593.	32.911	-29105.	-30873.	0.977
1700.	-1708645.	-1020378.	31.352	-28994.	-30928.	0.950
1750.	-1707104.	-1000157.	29.853	-28915.	-30986.	0.925
(2 sigma)	---	---	---	4113.	4111.	0.123
1800.	-1705566.	-979980.	28.438	-28871.	-31046.	0.901
(2 sigma)	---	---	---	4114.	4112.	0.119

Table 126. Thermophysical values for protoenstatite, $MgSiO_3$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
200.	62.755	53.053	-7089.	-88.500	32.2467
250.	72.809	68.199	-3686.	-82.944	32.2932
(2 sigma)	7.141	5.625	314.	4.755	0.1218
273.15	76.499	74.812	-1957.	-81.977	32.3147
298.15	79.990	81.665	0.	-81.665	32.3380
(2 sigma)	5.960	4.822	0.	4.822	0.1154
300.	80.231	82.161	148.	-81.667	32.3397
350.	85.998	94.979	4309.	-82.666	32.3862
400.	90.648	106.776	8730.	-84.952	32.4327
450.	94.499	117.682	13361.	-87.991	32.4792
500.	97.757	127.812	18170.	-91.472	32.5257
(2 sigma)	3.430	3.347	893.	4.424	0.0908
550.	100.560	137.263	23129.	-95.210	32.5721
600.	103.005	146.120	28220.	-99.088	32.6186
650.	105.162	154.452	33425.	-103.029	32.6651
700.	107.083	162.317	38732.	-106.986	32.7116
750.	108.809	169.765	44130.	-110.925	32.7581
(2 sigma)	2.726	2.515	1555.	3.815	0.0689
800.	110.371	176.838	49610.	-114.825	32.8046
850.	111.793	183.573	55165.	-118.673	32.8511
900.	113.094	190.000	60787.	-122.458	32.8976
950.	114.291	196.147	66472.	-126.176	32.9440
1000.	115.398	202.038	72215.	-129.823	32.9905
(2 sigma)	2.943	1.903	2077.	3.324	0.0661
1050.	116.424	207.693	78011.	-133.397	33.0370
1100.	117.380	213.132	83856.	-136.899	33.0835
1150.	118.272	218.369	89748.	-140.328	33.1300
1200.	119.109	223.421	95682.	-143.685	33.1765
1250.	119.894	228.299	101658.	-146.973	33.2230
(2 sigma)	3.336	1.463	2628.	2.920	0.0843
1257.400	120.006	229.007	102545.	-147.454	33.2299
1300.	120.634	233.016	107671.	-150.192	33.2695
1350.	121.332	237.582	113720.	-153.345	33.3159
1400.	121.992	242.007	119804.	-156.433	33.3624
1450.	122.619	246.298	125919.	-159.458	33.4089
1500.	123.213	250.466	132065.	-162.422	33.4554
(2 sigma)	3.716	1.272	3278.	2.578	0.1137
1550.	123.778	254.515	138240.	-165.328	33.5019
1600.	124.317	258.453	144442.	-168.177	33.5484
1650.	124.831	262.287	150671.	-170.971	33.5949
1700.	125.322	266.021	156925.	-173.712	33.6414
1750.	125.792	269.660	163203.	-176.401	33.6879
(2 sigma)	4.048	1.368	4042.	2.284	0.1479
1800.	126.243	273.210	169504.	-179.041	33.7343
(2 sigma)	4.108	1.415	4208.	2.231	0.1550

Table 127. Thermochemical properties of protoenstatite, $MgSiO_3$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-1530560.	-1476188.	385.541	-20003.	-22608.	5.905
250.	-1531361.	-1462496.	305.572	-19923.	-23272.	4.863
(2 sigma)	---	---	---	5580.	4850.	1.013
273.15	-1531637.	-1456106.	278.452	-19936.	-23582.	4.510
298.15	-1531885.	-1449182.	253.891	-19976.	-23914.	4.190
(2 sigma)	---	---	---	5502.	4746.	0.832
300.	-1531901.	-1448669.	252.235	-19980.	-23939.	4.168
350.	-1532259.	-1434766.	214.127	-20129.	-24588.	3.670
400.	-1532481.	-1420822.	185.540	-20349.	-25211.	3.292
450.	-1532599.	-1406857.	163.304	-20627.	-25802.	2.995
500.	-1532636.	-1392883.	145.513	-20958.	-26360.	2.754
(2 sigma)	---	---	---	5263.	4432.	0.463
550.	-1532609.	-1378909.	130.958	-21339.	-26882.	2.553
600.	-1532533.	-1364939.	118.828	-21767.	-27367.	2.383
650.	-1532421.	-1350977.	108.566	-22242.	-27815.	2.235
700.	-1532282.	-1337025.	99.770	-22763.	-28225.	2.106
750.	-1532127.	-1323083.	92.148	-23330.	-28595.	1.992
(2 sigma)	---	---	---	4993.	4219.	0.294
800.	-1531965.	-1309152.	85.479	-23943.	-28926.	1.889
850.	-1531802.	-1295232.	79.595	-25314.	-29213.	1.795
900.	-1531648.	-1281320.	74.366	-25596.	-29434.	1.708
950.	-1540434.	-1267146.	69.672	-25859.	-29640.	1.630
1000.	-1540244.	-1252767.	65.438	-26107.	-29832.	1.558
(2 sigma)	---	---	---	4722.	4128.	0.216
1050.	-1540055.	-1238398.	61.607	-26341.	-30013.	1.493
1100.	-1539870.	-1224037.	58.125	-26566.	-30182.	1.433
1150.	-1539691.	-1209685.	54.946	-26783.	-30342.	1.378
1200.	-1539518.	-1195341.	52.032	-26994.	-30492.	1.327
1250.	-1539353.	-1181004.	49.351	-27202.	-30634.	1.280
(2 sigma)	---	---	---	4503.	4105.	0.172
1257.400	-1539329.	-1178884.	48.973	-27233.	-30655.	1.273
1300.	-1539197.	-1166673.	46.877	-27409.	-30767.	1.236
1350.	-1539051.	-1152348.	44.587	-27616.	-30892.	1.195
1400.	-1664368.	-1134424.	42.326	-27825.	-31009.	1.157
1450.	-1663403.	-1115514.	40.185	-28037.	-31119.	1.121
1500.	-1662422.	-1096638.	38.188	-28255.	-31222.	1.087
(2 sigma)	---	---	---	4409.	4117.	0.143
1550.	-1661425.	-1077795.	36.321	-28479.	-31317.	1.055
1600.	-1660413.	-1058985.	34.572	-28711.	-31405.	1.025
1650.	-1659386.	-1040206.	32.930	-28952.	-31486.	0.997
1700.	-1708854.	-1021008.	31.372	-29203.	-31559.	0.970
1750.	-1707655.	-1000795.	29.872	-29466.	-31624.	0.944
(2 sigma)	---	---	---	4507.	4151.	0.124
1800.	-1706437.	-980616.	28.457	-29742.	-31682.	0.919
(2 sigma)	---	---	---	4554.	4160.	0.121

Table 128. Thermophysical values for forsterite, Mg_2SiO_4, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T	C_p°	S°	$H_T^\circ - H_{298}^\circ$	$[G_T^\circ - H_{298}^\circ]/T$	V°
K	J/(mol K)	J/(mol K)	J/mol	J/(mol K)	cm3/mol
200.	84.941	54.595	-10165.	-105.421	43.5534
250.	104.867	75.847	-5385.	-97.386	43.6002
(2 sigma)	0.185	3.633	11.	3.632	0.0406
273.15	111.759	85.443	-2875.	-95.969	43.6246
298.15	118.099	95.511	0.	-95.511	43.6527
(2 sigma)	0.297	3.632	0.	3.632	0.0203
300.	118.530	96.243	219.	-95.513	43.6548
350.	128.641	115.309	6410.	-96.996	43.7162
400.	136.515	133.020	13046.	-100.405	43.7832
450.	142.875	149.479	20036.	-104.955	43.8550
500.	148.153	164.814	27316.	-110.183	43.9308
(2 sigma)	0.568	3.629	85.	3.631	0.0751
550.	152.626	179.150	34838.	-115.808	44.0101
600.	156.482	192.599	42568.	-121.652	44.0923
650.	159.851	205.260	50478.	-127.602	44.1769
700.	162.828	217.218	58546.	-133.580	44.2637
750.	165.485	228.544	66755.	-139.536	44.3521
(2 sigma)	0.960	3.637	259.	3.628	0.0848
800.	167.875	239.301	75090.	-145.438	44.4421
850.	170.040	249.545	83539.	-151.263	44.5334
900.	172.014	259.321	92091.	-156.997	44.6257
950.	173.824	268.670	100738.	-162.630	44.7189
1000.	175.490	277.629	109471.	-168.158	44.8129
(2 sigma)	1.294	3.669	526.	3.627	0.0869
1050.	177.032	286.229	118285.	-173.577	44.9075
1100.	178.464	294.498	127173.	-178.887	45.0027
1150.	179.799	302.461	136130.	-184.087	45.0983
1200.	181.047	310.140	145151.	-189.181	45.1943
1250.	182.217	317.554	154233.	-194.168	45.2907
(2 sigma)	1.552	3.726	870.	3.630	0.1331
1300.	183.317	324.723	163372.	-199.052	45.3874
1350.	184.354	331.661	172564.	-203.836	45.4842
1400.	185.333	338.383	181806.	-208.522	45.5813
1450.	186.261	344.903	191096.	-213.113	45.6786
1500.	187.140	351.233	200431.	-217.612	45.7760
(2 sigma)	1.755	3.802	1274.	3.639	0.2080
1550.	187.976	357.383	209809.	-222.022	45.8735
1600.	188.771	363.363	219228.	-226.346	45.9712
1650.	189.530	369.184	228686.	-230.586	46.0689
1700.	190.254	374.853	238181.	-234.746	46.1667
1750.	190.946	380.378	247711.	-238.829	46.2645
(2 sigma)	1.919	3.893	1725.	3.653	0.2936
1800.	191.609	385.766	257275.	-242.836	46.3624
(2 sigma)	1.948	3.912	1821.	3.656	0.3114

Table 129. Thermochemical properties of forsterite, Mg_2SiO_4, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-2170703.	-2092666.	546.548	-59469.	-59581.	15.561
250.	-2172023.	-2072988.	433.127	-59522.	-59603.	12.453
(2 sigma)	---	---	---	7703.	7434.	1.553
273.15	-2172417.	-2063799.	394.661	-59550.	-59610.	11.399
298.15	-2172729.	-2053843.	359.824	-59583.	-59614.	10.444
(2 sigma)	---	---	---	7703.	7394.	1.295
300.	-2172748.	-2053105.	357.477	-59585.	-59614.	10.380
350.	-2173084.	-2033133.	303.428	-59655.	-59613.	8.897
400.	-2173143.	-2013134.	262.888	-59733.	-59602.	7.783
450.	-2172997.	-1993140.	231.357	-59821.	-59580.	6.916
500.	-2172697.	-1973170.	206.136	-59922.	-59548.	6.221
(2 sigma)	---	---	---	7703.	7268.	0.759
550.	-2172278.	-1953237.	185.503	-60040.	-59505.	5.651
600.	-2171772.	-1933346.	168.313	-60176.	-59451.	5.176
650.	-2171200.	-1913500.	153.771	-60334.	-59384.	4.772
700.	-2170586.	-1893700.	141.309	-60515.	-59305.	4.425
750.	-2169946.	-1873944.	130.513	-60722.	-59211.	4.124
(2 sigma)	---	---	---	7706.	7214.	0.502
800.	-2169297.	-1854232.	121.069	-60957.	-59103.	3.859
850.	-2168656.	-1834560.	112.738	-61933.	-58974.	3.624
900.	-2168035.	-1814925.	105.335	-61806.	-58803.	3.413
950.	-2185303.	-1794781.	98.684	-61646.	-58641.	3.224
1000.	-2184622.	-1774245.	92.677	-61458.	-58487.	3.055
(2 sigma)	---	---	---	7716.	7274.	0.380
1050.	-2183949.	-1753743.	87.244	-61245.	-58344.	2.902
1100.	-2183289.	-1733272.	82.306	-61012.	-58211.	2.764
1150.	-2182643.	-1712832.	77.799	-60762.	-58089.	2.638
1200.	-2182015.	-1692419.	73.669	-60497.	-57979.	2.524
1250.	-2181407.	-1672031.	69.870	-60221.	-57879.	2.419
(2 sigma)	---	---	---	7744.	7448.	0.311
1300.	-2180821.	-1651668.	66.365	-59937.	-57791.	2.322
1350.	-2180258.	-1631327.	63.120	-59647.	-57714.	2.233
1400.	-2430627.	-1603797.	59.838	-59353.	-57648.	2.151
1450.	-2428435.	-1574306.	56.713	-59058.	-57592.	2.075
1500.	-2426214.	-1544891.	53.798	-58764.	-57547.	2.004
(2 sigma)	---	---	---	7795.	7734.	0.269
1550.	-2423967.	-1515551.	51.074	-58472.	-57511.	1.938
1600.	-2421694.	-1486283.	48.522	-58186.	-57485.	1.877
1650.	-2419396.	-1457087.	46.128	-57907.	-57467.	1.819
1700.	-2467582.	-1427511.	43.862	-57636.	-57458.	1.765
1750.	-2465092.	-1396957.	41.697	-57376.	-57457.	1.715
(2 sigma)	---	---	---	7877.	8126.	0.243
1800.	-2462573.	-1366475.	39.654	-57128.	-57462.	1.668
(2 sigma)	---	---	---	7897.	8217.	0.238

Table 130. Thermophysical values for chrysotile, $Mg_3Si_2O_5(OH)_4$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
200.	196.745	127.091	-23420.	-244.190	107.0710
250.	240.970	175.972	-12426.	-225.676	107.1752
(2 sigma)	0.499	1.131	25.	1.127	1.2252
273.15	257.763	198.060	-6649.	-222.403	107.2234
298.15	273.858	221.342	0.	-221.342	107.2755
(2 sigma)	0.770	1.127	0.	1.127	1.2170
300.	274.975	223.039	508.	-221.347	107.2794
350.	301.883	267.524	14954.	-224.799	107.3836
400.	323.696	309.307	30611.	-232.779	107.4878
450.	341.730	348.506	47261.	-243.483	107.5921
500.	356.878	385.317	64736.	-255.844	107.6963
(2 sigma)	4.820	1.769	570.	1.149	1.3111
550.	369.766	419.952	82911.	-269.205	107.8005
600.	380.849	452.613	101683.	-283.141	107.9047
650.	390.464	483.485	120971.	-297.376	108.0089
700.	398.866	512.736	140709.	-311.723	108.1131
750.	406.253	540.512	160841.	-326.058	108.2174
(2 sigma)	7.300	3.987	2114.	1.515	1.6534
800.	412.782	566.944	181320.	-340.294	108.3216
850.	418.575	592.146	202107.	-354.373	108.4258
900.	423.734	616.220	223167.	-368.256	108.5300
950.	428.342	639.256	244471.	-381.918	108.6342
1000.	432.466	661.334	265993.	-395.340	108.7384
(2 sigma)	8.644	6.056	4000.	2.279	2.1321
1050.	436.163	682.525	287711.	-408.515	108.8427
1100.	439.482	702.893	309603.	-421.436	108.9469
1150.	442.463	722.496	331653.	-434.102	109.0511
1200.	445.142	741.385	353845.	-446.514	109.1553
1250.	447.548	759.606	376163.	-458.675	109.2595
(2 sigma)	10.842	7.777	6086.	3.141	2.6749

Table 131. Thermochemical properties of chrysotile, $Mg_3Si_2O_5(OH)_4$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-4470806.	-4178448.	1091.298	---	---	---
250.	-4477197.	-4104587.	857.606	---	---	---
(2 sigma)	---	---	---	---	---	---
273.15	-4479664.	-4069970.	778.302	-161073.	-140521.	26.872
298.15	-4482037.	-4032365.	706.453	-163105.	-138548.	24.273
(2 sigma)	---	---	---	11723.	11703.	2.050
300.	-4482201.	-4029575.	701.611	-163249.	-138396.	24.097
350.	-4486142.	-3953812.	590.074	-166897.	-133959.	19.992
400.	-4489252.	-3877544.	506.355	-249642.	-123225.	16.092
450.	-4491704.	-3800927.	441.200	-248426.	-107493.	12.477
500.	-4493634.	-3724067.	389.050	-246962.	-91910.	9.602
(2 sigma)	---	---	---	11775.	11688.	1.221
550.	-4495147.	-3647034.	346.366	-245309.	-76484.	7.264
600.	-4496331.	-3569878.	310.785	-243519.	-61214.	5.329
650.	-4497258.	-3492634.	280.671	-241633.	-46098.	3.704
700.	-4497991.	-3415327.	254.855	-239688.	-31129.	2.323
750.	-4498582.	-3337973.	232.477	-237714.	-16301.	1.135
(2 sigma)	---	---	---	12050.	11665.	0.812
800.	-4499080.	-3260582.	212.894	-235737.	-1605.	0.105
850.	-4499526.	-3183162.	195.613	-235205.	12979.	-0.798
900.	-4499957.	-3105717.	180.251	-232442.	27499.	-1.596
950.	-4527189.	-3027432.	166.460	-229603.	41863.	-2.302
1000.	-4527477.	-2948490.	154.013	-226710.	56076.	-2.929
(2 sigma)	---	---	---	12626.	11729.	0.613
1050.	-4527769.	-2869533.	142.751	-223781.	70143.	-3.489
1100.	-4528078.	-2790562.	132.513	-220832.	84070.	-3.992
1150.	-4528417.	-2711577.	123.164	-217876.	97863.	-4.445
1200.	-4528796.	-2632576.	114.593	-214928.	111528.	-4.855
1250.	-4529225.	-2553558.	106.707	-211998.	125070.	-5.226
(2 sigma)	---	---	---	13515.	12032.	0.503

Table 132. Thermophysical values for talc, $Mg_3Si_4O_{10}(OH)_2$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
200.	219.745	151.735	-27144.	-287.456	135.6673
250.	280.133	207.648	-14560.	-265.887	135.8134
(2 sigma)	1.203	1.339	45.	1.328	0.8281
273.15	302.061	233.436	-7815.	-262.046	135.8810
298.15	322.661	260.799	0.	-260.799	135.9541
(2 sigma)	0.739	1.328	0.	1.328	0.7568
300.	324.076	262.799	598.	-260.805	135.9595
350.	357.691	315.387	17677.	-264.881	136.1055
400.	384.318	364.953	36252.	-274.324	136.2516
450.	405.959	411.510	56026.	-287.007	136.3977
500.	423.895	455.239	76786.	-301.667	136.5437
(2 sigma)	0.792	1.356	109.	1.329	0.6206
550.	438.988	496.368	98368.	-317.516	136.6898
600.	451.844	535.131	120648.	-334.051	136.8358
650.	462.901	571.745	143523.	-350.940	136.9819
700.	472.489	606.409	166913.	-367.961	137.1280
750.	480.854	639.299	190751.	-384.963	137.2740
(2 sigma)	1.084	1.457	327.	1.340	0.8906
800.	488.193	670.572	214982.	-401.845	137.4201
850.	494.657	700.366	239556.	-418.535	137.5661
900.	500.371	728.805	264435.	-434.988	137.7122
950.	505.434	755.997	289582.	-451.173	137.8583
1000.	509.929	782.039	314969.	-467.070	138.0043
(2 sigma)	1.160	1.594	587.	1.364	1.3819
1050.	513.924	807.017	340567.	-482.667	138.1504
1100.	517.477	831.008	366354.	-497.959	138.2965
1150.	520.636	854.082	392308.	-512.945	138.4425
1200.	523.443	876.301	418412.	-527.625	138.5886
1250.	525.934	897.720	444647.	-542.003	138.7346
(2 sigma)	1.328	1.722	848.	1.400	1.9326

Table 133. Thermochemical properties of talc, $Mg_3Si_4O_{10}(OH)_2$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-6179020.	-5736774.	1498.291	---	---	---
250.	-6190709.	-5624813.	1175.239	---	---	---
(2 sigma)	---	---	---	---	---	---
273.15	-6195456.	-5572195.	1065.573	-161211.	-147018.	28.114
298.15	-6200218.	-5514937.	966.193	-162363.	-145667.	25.520
(2 sigma)	---	---	---	13080.	13043.	2.285
300.	-6200558.	-5510684.	959.495	-162444.	-145563.	25.345
350.	-6209141.	-5395011.	805.161	-164417.	-142589.	21.280
400.	-6216812.	-5278174.	689.258	-205850.	-136451.	17.819
450.	-6223807.	-5160418.	599.005	-205269.	-127810.	14.836
500.	-6230292.	-5041912.	526.725	-204572.	-119240.	12.457
(2 sigma)	---	---	---	13084.	13024.	1.361
550.	-6236395.	-4922776.	467.526	-203823.	-110743.	10.517
600.	-6242212.	-4803098.	418.146	-203069.	-102314.	8.907
650.	-6247823.	-4682943.	376.326	-202354.	-93947.	7.550
700.	-6253294.	-4562361.	340.447	-201712.	-85633.	6.390
750.	-6258678.	-4441392.	309.326	-201171.	-77361.	5.388
(2 sigma)	---	---	---	13094.	13006.	0.906
800.	-6264024.	-4320065.	282.071	-200755.	-69121.	4.513
850.	-6269373.	-4198404.	258.002	-203336.	-60882.	3.741
900.	-6274762.	-4076427.	236.590	-201540.	-52554.	3.050
950.	-6307002.	-3953334.	217.369	-199663.	-44328.	2.437
1000.	-6312351.	-3829319.	200.023	-197729.	-36202.	1.891
(2 sigma)	---	---	---	13109.	12997.	0.679
1050.	-6317752.	-3705035.	184.315	-195760.	-28174.	1.402
1100.	-6323217.	-3580492.	170.023	-193778.	-20241.	0.961
1150.	-6328757.	-3455698.	156.963	-191799.	-12397.	0.563
1200.	-6334381.	-3330663.	144.980	-189840.	-4639.	0.202
1250.	-6340096.	-3205391.	133.946	-187914.	3038.	-0.127
(2 sigma)	---	---	---	13129.	13000.	0.543

Table 134. Thermophysical values for anthophyllite, $Mg_7Si_8O_{22}(OH)_2$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
200.	476.042	309.014	-56657.	-592.298	263.7887
250.	582.722	427.172	-30082.	-547.499	263.8268
(2 sigma)	0.895	1.032	42.	1.021	2.5885
273.15	623.991	480.613	-16105.	-539.573	263.8445
298.15	663.615	537.004	0.	-537.004	263.8636
(2 sigma)	0.838	1.021	0.	1.021	2.5884
300.	666.361	541.118	1230.	-537.017	263.8650
350.	732.181	648.978	36258.	-545.384	263.9031
400.	784.583	750.297	74225.	-564.734	263.9412
450.	826.807	845.233	114547.	-590.684	263.9794
500.	861.200	934.186	156776.	-620.634	264.0175
(2 sigma)	1.212	1.116	181.	1.025	2.5883
550.	889.479	1017.636	200565.	-652.972	264.0556
600.	912.918	1096.067	245643.	-686.662	264.0938
650.	932.483	1169.935	291793.	-721.023	264.1319
700.	948.917	1239.659	338840.	-755.602	264.1700
750.	962.802	1305.614	386642.	-790.091	264.2081
(2 sigma)	2.474	1.324	461.	1.055	2.5897
800.	974.600	1368.138	435085.	-824.282	264.2463
850.	984.683	1427.533	484073.	-858.035	264.2844
900.	993.354	1484.068	533530.	-891.257	264.3225
950.	1000.863	1537.982	583390.	-923.887	264.3607
1000.	1007.416	1589.489	633600.	-955.889	264.3988
(2 sigma)	4.894	1.840	1202.	1.111	2.5927
1050.	1013.188	1638.784	684118.	-987.243	264.4369
1100.	1018.326	1686.038	734908.	-1017.940	264.4751
1150.	1022.955	1731.408	785942.	-1047.980	264.5132
1200.	1027.183	1775.036	837197.	-1077.371	264.5513
1250.	1031.102	1817.048	888655.	-1106.123	264.5895
(2 sigma)	6.230	2.782	2508.	1.236	2.5972

Table 135. Thermochemical properties of anthophyllite, $Mg_7Si_8O_{22}(OH)_2$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-12047331.	-11570007.	3021.774	---	---	---
250.	-12054571.	-11449759.	2392.294	---	---	---
(2 sigma)	---	---	---	---	---	---
273.15	-12056737.	-11393651.	2178.813	-277679.	-263848.	50.456
298.15	-12058366.	-11332884.	1985.473	-278531.	-262543.	45.996
(2 sigma)	---	---	---	29301.	29291.	5.132
300.	-12058460.	-11328382.	1972.445	-278588.	-262443.	45.695
350.	-12059770.	-11206568.	1672.488	-279854.	-259646.	38.750
400.	-12059098.	-11084707.	1447.513	-320451.	-253796.	33.142
450.	-12056902.	-10963026.	1272.554	-318962.	-245551.	28.503
500.	-12053539.	-10841655.	1132.619	-317355.	-237480.	24.809
(2 sigma)	---	---	---	29303.	29285.	3.059
550.	-12049290.	-10720666.	1018.163	-315760.	-229571.	21.803
600.	-12044384.	-10600095.	922.820	-314283.	-221802.	19.310
650.	-12039005.	-10479953.	842.179	-313015.	-214148.	17.209
700.	-12033310.	-10360237.	773.090	-312027.	-206582.	15.415
750.	-12027429.	-10240937.	713.242	-311382.	-199075.	13.865
(2 sigma)	---	---	---	29313.	29279.	2.039
800.	-12021471.	-10122031.	660.900	-311125.	-191598.	12.510
850.	-12015534.	-10003498.	614.740	-316995.	-184083.	11.312
900.	-12009700.	-9885312.	573.728	-314241.	-176344.	10.235
950.	-12066526.	-9765545.	536.947	-311444.	-168759.	9.279
1000.	-12060606.	-9644595.	503.782	-308646.	-161322.	8.427
(2 sigma)	---	---	---	29344.	29274.	1.529
1050.	-12054800.	-9523937.	473.790	-305881.	-154024.	7.662
1100.	-12049129.	-9403554.	446.537	-303175.	-146856.	6.974
1150.	-12043609.	-9283424.	421.666	-300550.	-139810.	6.350
1200.	-12038250.	-9163532.	398.878	-298024.	-132876.	5.784
1250.	-12033058.	-9043859.	377.922	-295609.	-126045.	5.267
(2 sigma)	---	---	---	29436.	29277.	1.223

Table 136. Thermophysical values for antigorite, $Mg_{48}Si_{34}O_{85}(OH)_{62}$, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
200.	3187.253	2079.151	-379417.	-3976.237	1745.6268
250.	3903.932	2871.061	-201307.	-3676.290	1747.4221
(2 sigma)	8.082	18.445	406.	18.387	12.7897
273.15	4175.912	3228.897	-107721.	-3623.263	1748.2533
298.15	4436.520	3606.080	0.	-3606.080	1749.1510
(2 sigma)	12.488	18.387	0.	18.387	12.7276
300.	4454.596	3633.579	8224.	-3606.164	1749.2174
350.	4890.106	4354.200	242243.	-3662.077	1751.0127
400.	5242.994	5031.003	495864.	-3791.343	1752.8080
450.	5534.599	5665.895	765525.	-3964.729	1754.6033
500.	5779.416	6262.055	1048546.	-4164.962	1756.3986
(2 sigma)	78.216	28.792	9257.	18.748	13.7113
550.	5987.621	6822.914	1342858.	-4381.355	1758.1939
600.	6166.575	7351.768	1646822.	-4607.065	1759.9892
650.	6321.739	7851.628	1959119.	-4837.598	1761.7845
700.	6457.258	8325.190	2278669.	-5069.948	1763.5798
750.	6576.337	8774.842	2604572.	-5302.080	1765.3751
(2 sigma)	118.420	64.752	34310.	24.672	17.1262
800.	6681.498	9202.695	2936071.	-5532.606	1767.1704
850.	6774.756	9610.612	3272523.	-5760.585	1768.9657
900.	6857.741	10000.241	3613376.	-5985.379	1770.7610
950.	6931.789	10373.041	3958149.	-6206.569	1772.5563
1000.	6998.004	10730.311	4306424.	-6423.887	1774.3517
(2 sigma)	140.061	98.307	64900.	37.059	21.8975
1050.	7057.311	11073.206	4657834.	-6637.174	1776.1470
1100.	7110.487	11402.762	5012053.	-6846.350	1777.9423
1150.	7158.194	11719.907	5368792.	-7051.393	1779.7376
1200.	7200.998	12025.478	5727791.	-7252.319	1781.5329
1250.	7239.385	12320.230	6088818.	-7449.175	1783.3282
(2 sigma)	175.420	126.177	98673.	51.027	27.3236

Table 137. Thermochemical properties of antigorite, $Mg_{48}Si_{34}O_{85}(OH)_{62}$, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
200.	-71308557.	-67838940.	17717.701	---	---	---
250.	-71364590.	-66964522.	13991.461	---	---	---
(2 sigma)	---	---	---	---	---	---
273.15	-71382546.	-66556233.	12727.580	-2683386.	-2367618.	452.761
298.15	-71397109.	-66113823.	11582.859	-2714846.	-2337300.	409.485
(2 sigma)	---	---	---	224232.	223907.	39.228
300.	-71398003.	-66081038.	11505.723	-2717079.	-2334951.	406.551
350.	-71413640.	-65193422.	9729.579	-2773515.	-2266706.	338.287
400.	-71415142.	-64304567.	8397.309	-4055953.	-2100871.	274.345
450.	-71405292.	-63416230.	7361.159	-4036981.	-1857579.	215.622
500.	-71386271.	-62529500.	6532.407	-4014194.	-1616614.	168.886
(2 sigma)	---	---	---	225291.	223600.	23.359
550.	-71359831.	-61645048.	5854.554	-3988543.	-1378078.	130.879
600.	-71327414.	-60763276.	5289.909	-3960830.	-1141973.	99.418
650.	-71290230.	-59884410.	4812.367	-3931732.	-908241.	72.987
700.	-71249313.	-59008553.	4403.269	-3901821.	-676783.	50.502
750.	-71205561.	-58135725.	4048.929	-3871584.	-447478.	31.165
(2 sigma)	---	---	---	230028.	222836.	15.520
800.	-71159767.	-57265887.	3739.076	-3841439.	-220189.	14.377
850.	-71112638.	-56398958.	3465.856	-3835959.	5405.	-0.332
900.	-71064814.	-55534825.	3223.155	-3792639.	230124.	-13.356
950.	-71445345.	-54660321.	3005.432	-3748118.	452402.	-24.875
1000.	-71394390.	-53778214.	2809.084	-3702733.	672311.	-35.118
(2 sigma)	---	---	---	239070.	222927.	11.644
1050.	-71343099.	-52898666.	2631.563	-3656777.	889934.	-44.272
1100.	-71291734.	-52021564.	2470.296	-3610512.	1105361.	-52.489
1150.	-71240518.	-51146795.	2323.159	-3564170.	1318681.	-59.896
1200.	-71189651.	-50274247.	2188.379	-3517959.	1529988.	-66.599
1250.	-71139306.	-49403808.	2064.471	-3472064.	1739374.	-72.684
(2 sigma)	---	---	---	252396.	226079.	9.447

Table 138. Thermophysical values for the element oxygen (O_2) at 1.01325 bars (1 atm). The sources of data are given in Section 1.5.5.

T	C_p°	S°	$H_T^\circ - H_{298}^\circ$	$[G_T^\circ - H_{298}^\circ]/T$	V°
K	J/(mol K)	J/(mol K)	J/mol	J/(mol K)	cm3/mol
200.	29.198	193.397	-2861.	-207.702	---
250.	29.087	199.888	-1407.	-205.514	---
(2 sigma)	---	---	---	---	---
273.15	29.199	202.468	-732.	-205.148	---
298.15	29.377	205.033	-0.	-205.033	---
(2 sigma)	---	---	---	---	---
300.	29.391	205.214	54.	-205.033	---
350.	29.836	209.778	1535.	-205.393	---
400.	30.320	213.793	3039.	-206.197	---
450.	30.805	217.392	4567.	-207.244	---
500.	31.274	220.662	6119.	-208.425	---
(2 sigma)	---	---	---	---	---
550.	31.722	223.664	7694.	-209.676	---
600.	32.145	226.443	9291.	-210.959	---
650.	32.545	229.032	10908.	-212.250	---
700.	32.921	231.457	12545.	-213.537	---
750.	33.275	233.741	14200.	-214.808	---
(2 sigma)	---	---	---	---	---
800.	33.607	235.899	15872.	-216.059	---
850.	33.919	237.946	17560.	-217.287	---
900.	34.212	239.893	19263.	-218.489	---
950.	34.487	241.750	20981.	-219.665	---
1000.	34.744	243.526	22712.	-220.814	---
(2 sigma)	---	---	---	---	---
1050.	34.985	245.227	24455.	-221.936	---
1100.	35.209	246.860	26210.	-223.032	---
1150.	35.419	248.429	27976.	-224.103	---
1200.	35.613	249.941	29752.	-225.148	---
1250.	35.793	251.399	31537.	-226.169	---
(2 sigma)	---	---	---	---	---
1300.	35.960	252.806	33331.	-227.167	---
1350.	36.112	254.166	35133.	-228.142	---
1400.	36.252	255.482	36942.	-229.095	---
1450.	36.378	256.756	38757.	-230.027	---
1500.	36.492	257.991	40579.	-230.938	---
(2 sigma)	---	---	---	---	---
1550.	36.594	259.189	42406.	-231.830	---
1600.	36.683	260.353	44238.	-232.704	---
1650.	36.760	261.483	46075.	-233.559	---
1700.	36.826	262.581	47914.	-234.396	---
1750.	36.880	263.649	49757.	-235.217	---
(2 sigma)	---	---	---	---	---
1800.	36.922	264.689	51602.	-236.021	---
(2 sigma)	---	---	---	---	---

Table 139. Thermochemical properties of the element oxygen (O_2) at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
200.	0.	0.	0.	---	---	---
250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
273.15	0.	0.	0.	---	---	---
298.15	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
300.	0.	0.	0.	---	---	---
350.	0.	0.	0.	---	---	---
400.	0.	0.	0.	---	---	---
450.	0.	0.	0.	---	---	---
500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
550.	0.	0.	0.	---	---	---
600.	0.	0.	0.	---	---	---
650.	0.	0.	0.	---	---	---
700.	0.	0.	0.	---	---	---
750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
800.	0.	0.	0.	---	---	---
850.	0.	0.	0.	---	---	---
900.	0.	0.	0.	---	---	---
950.	0.	0.	0.	---	---	---
1000.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1050.	0.	0.	0.	---	---	---
1100.	0.	0.	0.	---	---	---
1150.	0.	0.	0.	---	---	---
1200.	0.	0.	0.	---	---	---
1250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1300.	0.	0.	0.	---	---	---
1350.	0.	0.	0.	---	---	---
1400.	0.	0.	0.	---	---	---
1450.	0.	0.	0.	---	---	---
1500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1550.	0.	0.	0.	---	---	---
1600.	0.	0.	0.	---	---	---
1650.	0.	0.	0.	---	---	---
1700.	0.	0.	0.	---	---	---
1750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1800.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---

Table 140. Thermophysical values for stable phases of the element silicon (Si) at 1.01325 bars (1 atm). The sources of data are given in Section 1.5.5.

T	C_p°	S°	$H_T^\circ - H_{298}^\circ$	$[G_T^\circ - H_{298}^\circ]/T$	V°
K	J/(mol K)	J/(mol K)	J/mol	J/(mol K)	cm3/mol
		silicon (crystal)			
200.	15.588	11.648	-1775.	-20.521	---
250.	18.271	15.440	-923.	-19.130	---
(2 sigma)	---	---	---	---	---
273.15	19.154	17.097	-489.	-18.888	---
298.15	19.946	18.810	0.	-18.810	---
(2 sigma)	---	---	---	---	---
300.	19.999	18.934	37.	-18.810	---
350.	21.222	22.113	1069.	-19.059	---
400.	22.146	25.010	2154.	-19.624	---
450.	22.875	27.662	3280.	-20.372	---
500.	23.470	30.104	4439.	-21.225	---
(2 sigma)	---	---	---	---	---
550.	23.970	32.365	5626.	-22.136	---
600.	24.398	34.469	6835.	-23.077	---
650.	24.771	36.437	8065.	-24.030	---
700.	25.100	38.285	9312.	-24.983	---
750.	25.394	40.027	10574.	-25.928	---
(2 sigma)	---	---	---	---	---
800.	25.659	41.675	11851.	-26.861	---
850.	25.901	43.238	13140.	-27.779	---
900.	26.122	44.724	14440.	-28.680	---
950.	26.327	46.142	15752.	-29.562	---
1000.	26.517	47.498	17073.	-30.425	---
(2 sigma)	---	---	---	---	---
1050.	26.693	48.796	18403.	-31.269	---
1100.	26.859	50.041	19742.	-32.094	---
1150.	27.015	51.239	21089.	-32.901	---
1200.	27.162	52.392	22443.	-33.689	---
1250.	27.302	53.503	23805.	-34.459	---
(2 sigma)	---	---	---	---	---
1300.	27.435	54.577	25173.	-35.213	---
1350.	27.561	55.614	26548.	-35.949	---
1400.	27.682	56.619	27929.	-36.669	---
1450.	27.797	57.592	29316.	-37.374	---
1500.	27.908	58.537	30709.	-38.064	---
(2 sigma)	---	---	---	---	---
1550.	28.015	59.454	32107.	-38.739	---
1600.	28.118	60.345	33510.	-39.401	---
1650.	28.217	61.211	34919.	-40.048	---
1685.	28.285	61.804	35908.	-40.494	---
		silicon (liquid)			
1685.	25.522	91.805	86459.	-40.494	---
1700.	25.522	92.031	86841.	-40.948	---
1750.	25.522	92.771	88117.	-42.418	---
(2 sigma)	---	---	---	---	---
1800.	25.522	93.490	89394.	-43.827	---
(2 sigma)	---	---	---	---	---

Table 141. Thermochemical properties of stable phases of the element silicon (Si) at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
			silicon (crystal)			
200.	0.	0.	0.	---	---	---
250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
273.15	0.	0.	0.	---	---	---
298.15	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
300.	0.	0.	0.	---	---	---
350.	0.	0.	0.	---	---	---
400.	0.	0.	0.	---	---	---
450.	0.	0.	0.	---	---	---
500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
550.	0.	0.	0.	---	---	---
600.	0.	0.	0.	---	---	---
650.	0.	0.	0.	---	---	---
700.	0.	0.	0.	---	---	---
750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
800.	0.	0.	0.	---	---	---
850.	0.	0.	0.	---	---	---
900.	0.	0.	0.	---	---	---
950.	0.	0.	0.	---	---	---
1000.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1050.	0.	0.	0.	---	---	---
1100.	0.	0.	0.	---	---	---
1150.	0.	0.	0.	---	---	---
1200.	0.	0.	0.	---	---	---
1250.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1300.	0.	0.	0.	---	---	---
1350.	0.	0.	0.	---	---	---
1400.	0.	0.	0.	---	---	---
1450.	0.	0.	0.	---	---	---
1500.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1550.	0.	0.	0.	---	---	---
1600.	0.	0.	0.	---	---	---
1650.	0.	0.	0.	---	---	---
1685.	0.	0.	0.	---	---	---
			silicon (liquid)			
1685.	0.	0.	0.	---	---	---
1700.	0.	0.	0.	---	---	---
1750.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---
1800.	0.	0.	0.	---	---	---
(2 sigma)	0.	0.	0.	---	---	---

Table 142. Thermophysical values for quartz, SiO_2, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T K	C_p° J/(mol K)	S° J/(mol K)	$H_T^\circ - H_{298}^\circ$ J/mol	$[G_T^\circ - H_{298}^\circ]/T$ J/(mol K)	V° cm3/mol
		alpha quartz			
200.	32.629	26.024	-3846.	-45.251	22.4533
250.	39.535	34.083	-2033.	-42.216	22.5212
(2 sigma)	---	---	---	---	---
273.15	42.175	37.701	-1087.	-41.681	22.5526
298.15	44.741	41.507	0.	-41.507	22.5865
(2 sigma)	---	---	---	---	---
300.	44.921	41.785	83.	-41.508	22.5890
350.	49.351	49.052	2443.	-42.072	22.6569
400.	53.136	55.895	5007.	-43.376	22.7248
450.	56.459	62.349	7749.	-45.129	22.7926
500.	59.439	68.454	10648.	-47.159	22.8605
(2 sigma)	---	---	---	---	---
550.	62.156	74.249	13688.	-49.361	22.9283
600.	64.667	79.766	16860.	-51.667	22.9962
650.	67.011	85.036	20152.	-54.032	23.0641
700.	69.219	90.083	23559.	-56.428	23.1319
750.	71.314	94.931	27072.	-58.835	23.1998
(2 sigma)	---	---	---	---	---
800.	73.314	99.598	30688.	-61.237	23.2677
844.	75.007	103.568	33952.	-63.341	23.3274
		beta quartz			
844.	67.386	104.467	35287.	-62.657	23.5794
850.	67.446	104.944	35692.	-62.954	23.5794
900.	67.948	108.814	39076.	-65.395	23.5794
950.	68.450	112.501	42486.	-67.778	23.5794
1000.	68.952	116.025	45921.	-70.103	23.5794
(2 sigma)	---	---	---	---	---
1050.	69.454	119.401	49382.	-72.371	23.5794
1100.	69.956	122.644	52867.	-74.583	23.5794
1150.	70.458	125.764	56377.	-76.741	23.5794
1200.	70.960	128.774	59913.	-78.846	23.5794
1250.	71.462	131.681	63473.	-80.902	23.5794
(2 sigma)	---	---	---	---	---
1300.	71.964	134.493	67059.	-82.909	23.5794
1350.	72.466	137.219	70670.	-84.871	23.5794
1400.	72.968	139.863	74306.	-86.788	23.5794
1450.	73.470	142.432	77967.	-88.662	23.5794
1500.	73.972	144.932	81653.	-90.497	23.5794
(2 sigma)	---	---	---	---	---
1550.	74.474	147.365	85364.	-92.292	23.5794
1600.	74.976	149.738	89100.	-94.050	23.5794
1650.	75.478	152.052	92861.	-95.773	23.5794
1700.	75.980	154.313	96648.	-97.462	23.5794
1750.	76.482	156.523	100459.	-99.118	23.5794
(2 sigma)	---	---	---	---	---
1800.	76.984	158.684	104296.	-100.742	23.5794
(2 sigma)	---	---	---	---	---

Table 143. Thermochemical properties of quartz, SiO_2, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T	$\Delta H^\circ_{f,e}$	$\Delta G^\circ_{f,e}$	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$	$\Delta G^\circ_{f,ox}$	log $K^\circ_{f,ox}$
K	J/mol	J/mol		J/mol	J/mol	
			alpha quartz			
200.	-909880.	-874075.	228.285	0.0	0.0	0.0
250.	-910374.	-865063.	180.745	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
273.15	-910536.	-860859.	164.623	0.0	0.0	0.0
298.15	-910670.	-856306.	150.021	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
300.	-910678.	-855969.	149.037	0.0	0.0	0.0
350.	-910831.	-846837.	126.383	0.0	0.0	0.0
400.	-910855.	-837692.	109.391	0.0	0.0	0.0
450.	-910768.	-828551.	96.176	0.0	0.0	0.0
500.	-910581.	-819425.	85.605	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
550.	-910301.	-810322.	76.958	0.0	0.0	0.0
600.	-909936.	-801248.	69.755	0.0	0.0	0.0
650.	-909490.	-792209.	63.663	0.0	0.0	0.0
700.	-908968.	-783206.	58.444	0.0	0.0	0.0
750.	-908371.	-774243.	53.923	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
800.	-907704.	-765323.	49.970	0.0	0.0	0.0
844.	-907059.	-757509.	46.882	0.0	0.0	0.0
			beta quartz			
844.	-906301.	-757509.	46.882	0.0	0.0	0.0
850.	-906255.	-756452.	46.486	0.0	0.0	0.0
900.	-905874.	-747651.	43.392	0.0	0.0	0.0
950.	-905493.	-738871.	40.626	0.0	0.0	0.0
1000.	-905110.	-730111.	38.137	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1050.	-904723.	-721371.	35.886	0.0	0.0	0.0
1100.	-904332.	-712649.	33.841	0.0	0.0	0.0
1150.	-903934.	-703945.	31.974	0.0	0.0	0.0
1200.	-903529.	-695258.	30.264	0.0	0.0	0.0
1250.	-903115.	-686589.	28.691	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1300.	-902692.	-677936.	27.240	0.0	0.0	0.0
1350.	-902258.	-669300.	25.897	0.0	0.0	0.0
1400.	-901812.	-660680.	24.650	0.0	0.0	0.0
1450.	-901354.	-652076.	23.490	0.0	0.0	0.0
1500.	-900883.	-643488.	22.408	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1550.	-900397.	-634916.	21.397	0.0	0.0	0.0
1600.	-899896.	-626360.	20.449	0.0	0.0	0.0
1650.	-899379.	-617820.	19.559	0.0	0.0	0.0
1700.	-949355.	-608846.	18.708	0.0	0.0	0.0
1750.	-948662.	-598841.	17.874	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0
1800.	-947947.	-588857.	17.088	0.0	0.0	0.0
(2 sigma)	---	---	---	0.0	0.0	0.0

Table 144. Thermophysical values for cristobalite, SiO_2, at 1.01325 bars (1 atm). The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

T	C_p°	S°	$H_T^\circ - H_{298}^\circ$	$[G_T^\circ - H_{298}^\circ]/T$	V°
K	J/(mol K)	J/(mol K)	J/mol	J/(mol K)	cm3/mol
		alpha cristobalite			
200.	32.999	29.306	-3873.	-48.671	25.5527
250.	39.806	37.435	-2045.	-45.616	25.6816
(2 sigma)	---	---	---	---	0.0790
273.15	42.421	41.077	-1093.	-45.077	25.7412
298.15	44.961	44.903	0.	-44.903	25.8057
(2 sigma)	---	---	---	---	0.0574
300.	45.139	45.182	83.	-44.904	25.8104
350.	49.484	52.477	2452.	-45.470	25.9393
400.	53.110	59.328	5020.	-46.779	26.0682
450.	56.174	65.766	7754.	-48.534	26.1970
500.	58.779	71.823	10630.	-50.563	26.3259
(2 sigma)	---	---	---	---	0.0694
523.	59.844	74.490	11994.	-51.557	26.3851
523.	58.312	77.016	13315.	-51.557	27.3414
550.	59.797	79.989	14910.	-52.880	27.3471
600.	62.048	85.292	17958.	-55.362	27.3577
650.	63.813	90.331	21106.	-57.860	27.3683
700.	65.228	95.114	24334.	-60.352	27.3789
750.	66.381	99.655	27625.	-62.822	27.3895
(2 sigma)	---	---	---	---	0.0573
800.	67.337	103.970	30968.	-65.260	27.4001
850.	68.140	108.078	34356.	-67.659	27.4107
900.	68.824	111.992	37781.	-70.014	27.4213
950.	69.412	115.729	41237.	-72.322	27.4319
1000.	69.924	119.303	44720.	-74.583	27.4425
(2 sigma)	---	---	---	---	0.0604
1050.	70.373	122.726	48228.	-76.794	27.4531
1100.	70.771	126.009	51757.	-78.957	27.4637
1150.	71.126	129.163	55304.	-81.072	27.4743
1200.	71.446	132.197	58869.	-83.139	27.4849
1250.	71.736	135.119	62449.	-85.160	27.4955
(2 sigma)	---	---	---	---	0.0884
1300.	72.000	137.938	66042.	-87.136	27.5061
1350.	72.243	140.660	69648.	-89.069	27.5167
1400.	72.466	143.291	73266.	-90.959	27.5273
1450.	72.674	145.838	76895.	-92.807	27.5378
1500.	72.867	148.305	80533.	-94.616	27.5484
(2 sigma)	---	---	---	---	0.1255
1550.	73.048	150.697	84181.	-96.387	27.5590
1600.	73.219	153.019	87838.	-98.121	27.5696
1650.	73.380	155.275	91503.	-99.819	27.5802
1700.	73.532	157.468	95176.	-101.482	27.5908
1750.	73.677	159.601	98856.	-103.112	27.6014
(2 sigma)	---	---	---	---	0.1658
1800.	73.816	161.679	102543.	-104.710	27.6120
(2 sigma)	---	---	---	---	0.1740

Table 145. Thermochemical properties of cristobalite, SiO_2, at 1.01325 bars (1 atm). Columns 2 through 4 give the thermochemical values relative to the elements; columns 5 through 7 give the values relative to the oxides.

	Formation from the Elements			Formation from the Oxides		
T K	$\Delta H^\circ_{f,e}$ J/mol	$\Delta G^\circ_{f,e}$ J/mol	log $K^\circ_{f,e}$	$\Delta H^\circ_{f,ox}$ J/mol	$\Delta G^\circ_{f,ox}$ J/mol	log $K^\circ_{f,ox}$
		alpha cristobalite				
200.	-907133.	-871985.	227.739	0.	0.	0.
250.	-907611.	-863138.	180.343	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
273.15	-907767.	-859013.	164.269	0.	0.	0.
298.15	-907895.	-854545.	149.713	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
300.	-907903.	-854213.	148.732	0.	0.	0.
350.	-908047.	-845252.	126.147	0.	0.	0.
400.	-908068.	-836278.	109.207	0.	0.	0.
450.	-907988.	-827309.	96.031	0.	0.	0.
500.	-907824.	-818352.	85.493	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
523.	-907724.	-814239.	81.322	0.	0.	0.
		beta cristobalite				
523.	-906403.	-814239.	81.322	0.	0.	0.
550.	-906305.	-809483.	76.878	0.	0.	0.
600.	-906063.	-800691.	69.706	0.	0.	0.
650.	-905762.	-791922.	63.640	0.	0.	0.
700.	-905418.	-783178.	58.441	0.	0.	0.
750.	-905044.	-774459.	53.938	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
800.	-904649.	-765767.	49.999	0.	0.	0.
850.	-904239.	-757099.	46.526	0.	0.	0.
900.	-903818.	-748456.	43.439	0.	0.	0.
950.	-903391.	-739836.	40.679	0.	0.	0.
1000.	-902959.	-731239.	38.196	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
1050.	-902525.	-722664.	35.951	0.	0.	0.
1100.	-902090.	-714109.	33.910	0.	0.	0.
1150.	-901655.	-705574.	32.048	0.	0.	0.
1200.	-901221.	-697058.	30.342	0.	0.	0.
1250.	-900788.	-688560.	28.773	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
1300.	-900357.	-680080.	27.326	0.	0.	0.
1350.	-899928.	-671616.	25.986	0.	0.	0.
1400.	-899500.	-663167.	24.743	0.	0.	0.
1450.	-899075.	-654735.	23.586	0.	0.	0.
1500.	-898650.	-646316.	22.507	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
1550.	-898228.	-637912.	21.497	0.	0.	0.
1600.	-897806.	-629522.	20.552	0.	0.	0.
1650.	-897386.	-621144.	19.664	0.	0.	0.
1700.	-947475.	-612330.	18.815	0.	0.	0.
1750.	-946914.	-602481.	17.983	0.	0.	0.
(2 sigma)	---	---	---	0.	0.	0.
1800.	-946348.	-592648.	17.198			
(2 sigma)	---	---	---			

Table 146. Molar volume in cm^3/g of boehmite, AlOOH, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	19.54	19.84	20.14	20.44	21.04	21.65	---	---
500.	19.52	19.83	20.13	20.43	21.03	21.63	---	---
1000.	19.51	19.81	20.11	20.41	21.01	21.62	---	---
2000.	19.48	19.78	20.08	20.38	20.98	21.59	---	---
4000.	19.42	19.72	20.02	20.32	20.92	21.53	---	---
6000.	19.36	19.66	19.96	20.26	20.86	21.47	---	---
8000.	19.30	19.60	19.90	20.20	20.80	21.41	---	---
10000.	19.24	19.54	19.84	20.14	20.74	21.35	---	---

Table 147. Molar volume in cm^3/g of diaspore, AlOOH, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	17.76	17.88	18.00	18.12	18.36	18.59	19.07	19.55
500.	17.74	17.86	17.98	18.10	18.34	18.58	19.05	19.53
1000.	17.72	17.84	17.96	18.08	18.32	18.56	19.03	19.51
2000.	17.69	17.81	17.93	18.05	18.28	18.52	19.00	19.47
4000.	17.61	17.73	17.85	17.97	18.21	18.45	18.92	19.40
6000.	17.54	17.66	17.78	17.90	18.14	18.37	18.85	19.33
8000.	17.47	17.59	17.71	17.83	18.06	18.30	18.78	19.25
10000.	17.39	17.51	17.63	17.75	17.99	18.23	18.70	19.18

Table 148. Molar volume in cm^3/g of gibbsite, $Al(OH)_3$, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	31.96	32.01	32.06	32.12	32.23	32.33	---	---
500.	31.96	32.01	32.06	32.12	32.23	32.33	---	---
1000.	31.96	32.01	32.06	32.12	32.23	32.33	---	---
2000.	31.95	32.01	32.06	32.12	32.22	32.33	---	---
4000.	31.95	32.01	32.06	32.12	32.22	32.33	---	---
6000.	31.95	32.01	32.06	32.11	32.22	32.33	---	---
8000.	31.95	32.01	32.06	32.11	32.22	32.33	---	---
10000.	31.95	32.00	32.06	32.11	32.22	32.33	---	---

Table 149. Molar volume in cm^3/g of corundum, Al_2O_3, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	25.60	25.67	25.73	25.80	25.93	26.06	26.32	26.58
500.	25.59	25.66	25.72	25.79	25.92	26.05	26.31	26.58
1000.	25.59	25.65	25.72	25.78	25.92	26.05	26.31	26.57
2000.	25.58	25.64	25.71	25.77	25.90	26.04	26.30	26.56
4000.	25.55	25.62	25.68	25.75	25.88	26.01	26.27	26.54
6000.	25.53	25.60	25.66	25.73	25.86	25.99	26.25	26.51
8000.	25.51	25.58	25.64	25.71	25.84	25.97	26.23	26.49
10000.	25.49	25.55	25.62	25.69	25.82	25.95	26.21	26.47

Table 150. Molar volume in cm^3/g of andalusite, Al_2SiO_5, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	51.56	51.68	51.81	51.96	52.27	52.60	53.28	53.97
500.	51.54	51.66	51.79	51.94	52.25	52.58	53.26	53.95
1000.	51.52	51.64	51.77	51.91	52.23	52.56	53.24	53.93
2000.	51.47	51.59	51.73	51.87	52.18	52.51	53.19	53.89
4000.	51.39	51.51	51.64	51.79	52.10	52.43	53.11	53.80
6000.	51.31	51.43	51.56	51.71	52.02	52.35	53.03	53.72
8000.	51.23	51.35	51.48	51.63	51.94	52.27	52.95	53.64
10000.	51.15	51.27	51.40	51.55	51.86	52.19	52.87	53.56

Table 151. Molar volume in cm^3/g of kyanite, Al_2SiO_5, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	44.21	44.31	44.42	44.53	44.76	45.01	45.50	46.00
500.	44.19	44.29	44.40	44.51	44.75	44.99	45.48	45.98
1000.	44.17	44.28	44.39	44.50	44.73	44.97	45.47	45.97
2000.	44.14	44.25	44.35	44.47	44.70	44.94	45.44	45.93
4000.	44.08	44.19	44.30	44.41	44.64	44.88	45.38	45.88
6000.	44.03	44.13	44.24	44.35	44.59	44.83	45.32	45.82
8000.	43.98	44.08	44.19	44.30	44.54	44.78	45.27	45.77
10000.	43.93	44.03	44.14	44.25	44.49	44.73	45.22	45.72

Table 152. Molar volume in cm^3/g of sillimanite, Al_2SiO_5, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	50.02	50.07	50.13	50.20	50.36	50.53	50.90	51.27
500.	50.00	50.05	50.11	50.18	50.34	50.51	50.88	51.25
1000.	49.98	50.03	50.09	50.16	50.32	50.49	50.86	51.23
2000.	49.94	49.99	50.05	50.12	50.28	50.46	50.82	51.19
4000.	49.87	49.92	49.98	50.05	50.21	50.38	50.74	51.11
6000.	49.79	49.84	49.90	49.97	50.13	50.31	50.67	51.04
8000.	49.72	49.77	49.83	49.90	50.06	50.23	50.60	50.97
10000.	49.65	49.70	49.76	49.83	49.99	50.16	50.52	50.89

Table 153. Molar volume in cm^3/g of kaolinite, $Al_2Si_2O_5(OH)_4$, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	99.48	99.84	100.20	100.55	101.26	101.98	103.40	104.82
500.	99.28	99.64	100.00	100.35	101.06	101.77	103.20	104.62
1000.	99.08	99.44	99.79	100.15	100.86	101.57	103.00	104.42
2000.	98.67	99.03	99.39	99.74	100.46	101.17	102.59	104.01
4000.	97.86	98.22	98.58	98.94	99.66	100.36	101.78	103.21
6000.	97.05	97.42	97.77	98.13	98.84	99.55	100.97	102.40
8000.	96.24	96.61	96.96	96.32	98.03	98.74	100.16	101.59
10000.	93.44	93.80	96.15	96.51	97.22	97.93	99.36	100.78

Table 154. Molar volume in cm^3/g of dickite, $Al_2Si_2O_5(OH)_4$, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	99.30	99.68	100.05	100.42	101.16	101.90	---	---
500.	99.10	99.48	99.85	100.22	100.96	101.70	---	---
1000.	98.90	99.28	99.65	100.02	100.76	101.50	---	---
2000.	98.50	98.88	99.25	99.62	100.36	101.10	---	---
4000.	97.70	98.08	98.45	98.82	99.56	100.30	---	---
6000.	96.90	97.28	97.65	98.02	98.76	99.50	---	---
8000.	96.10	96.48	96.85	97.22	97.96	98.70	---	---
10000.	95.30	95.68	96.05	96.42	97.16	97.90	---	---

Table 155. Molar volume in cm^3/g of halloysite, $Al_2Si_2O_5(OH)_4$, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	99.40	99.78	100.15	100.52	101.26	102.00	---	---
500.	99.20	99.58	99.95	100.32	101.06	101.80	---	---
1000.	99.00	99.38	99.75	100.12	100.86	101.60	---	---
2000.	98.60	98.98	99.35	99.72	100.46	101.20	---	---
4000.	97.80	98.18	98.55	98.92	99.66	100.40	---	---
6000.	97.00	97.38	97.75	98.12	98.86	99.60	---	---
8000.	96.20	96.58	96.95	97.32	98.06	98.80	---	---
10000.	95.40	95.78	96.15	96.52	97.26	98.00	---	---

Table 156. Molar volume in cm^3/g of pyrophyllite, $Al_2Si_4O_{10}(OH)_2$, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	127.64	127.73	127.84	127.97	128.26	128.58	---	---
500.	127.63	127.72	127.83	127.96	128.26	128.58	---	---
1000.	127.63	127.72	127.83	127.96	128.25	128.57	---	---
2000.	127.62	127.71	127.82	127.95	128.25	128.56	---	---
4000.	127.61	127.70	127.81	127.94	128.23	128.55	---	---
6000.	127.59	127.68	127.80	127.92	128.22	128.54	---	---
8000.	127.58	127.67	127.78	127.91	128.20	128.52	---	---
10000.	127.56	127.65	127.77	127.90	128.19	128.51	---	---

Table 157. Molar volume in cm^3/g of Ca-Al clinopyroxene, $CaAl_2SiO_6$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	63.58	63.72	63.88	64.04	64.39	64.75	65.50	66.26
500.	63.55	63.70	63.85	64.02	64.37	64.73	65.48	66.23
1000.	63.53	63.67	63.83	63.99	64.34	64.71	65.45	66.21
2000.	63.48	63.62	63.78	63.94	64.29	64.66	65.40	66.16
4000.	63.38	63.53	63.68	63.85	64.20	64.56	65.31	66.06
6000.	63.28	63.43	63.58	63.75	64.10	64.46	65.21	65.96
8000.	63.19	63.33	63.49	63.65	64.00	64.36	65.11	65.87
10000.	63.09	63.23	63.39	63.55	63.90	64.27	65.01	65.77

Table 158. Molar volume in cm^3/g of anorthite, $CaAl_2Si_2O_8$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	100.73	100.86	100.99	101.11	101.37	101.63	102.14	102.65
500.	100.66	100.79	100.92	101.05	101.30	101.56	102.07	102.59
1000.	100.60	100.73	100.85	100.98	101.24	101.50	102.01	102.52
2000.	100.46	100.59	100.72	100.85	101.11	101.36	101.88	102.39
4000.	100.20	100.33	100.46	100.59	100.85	101.10	101.62	102.13
6000.	99.95	100.08	100.20	100.33	100.59	100.84	101.36	101.87
8000.	99.69	99.82	99.95	100.08	100.33	100.59	101.10	101.61
10000.	99.43	99.57	99.69	99.82	100.08	100.33	100.85	101.36

Table 159. Molar volume in cm^3/g of margarite, $CaAl_4Si_2O_{10}(OH)_2$, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	133.77	134.08	134.39	134.69	135.30	135.91	---	---
500.	133.59	133.90	134.20	134.51	135.12	135.73	---	---
1000.	133.40	133.71	134.02	134.32	134.93	135.54	---	---
2000.	133.04	133.35	133.65	133.96	134.57	135.17	---	---
4000.	132.30	132.61	132.92	133.22	133.83	134.44	---	---
6000.	131.57	131.88	132.18	132.49	133.10	133.70	---	---
8000.	130.83	131.14	131.45	131.75	132.36	132.97	---	---
10000.	130.10	130.41	130.71	131.02	131.62	132.23	---	---

Table 160. Molar volume in cm^3/g of calcite, $CaCO_3$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	36.78	36.79	36.81	36.83	36.88	36.93	37.02	37.12
500.	36.75	36.77	36.79	36.81	36.85	36.90	37.00	37.10
1000.	36.72	36.74	36.76	36.78	36.82	36.87	36.97	37.07
2000.	36.67	36.69	36.70	36.72	36.77	36.82	36.92	37.02
4000.	36.56	36.58	36.60	36.62	36.66	36.71	36.81	36.91
6000.	36.46	36.47	36.49	36.51	36.56	36.61	36.70	36.80
8000.	36.35	36.37	36.39	36.41	36.45	36.50	36.60	36.70
10000.	36.25	36.27	36.29	36.31	36.35	36.40	36.50	36.60

Table 161. Molar volume in cm^3/g of aragonite, $CaCO_3$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	34.14	34.14	34.15	34.15	34.16	34.16	34.18	34.19
500.	34.14	34.14	34.15	34.15	34.16	34.16	34.18	34.19
1000.	34.14	34.14	34.14	34.15	34.15	34.16	34.17	34.19
2000.	34.13	34.13	34.14	34.14	34.14	34.15	34.16	34.18
4000.	34.09	34.10	34.10	34.10	34.11	34.11	34.13	34.14
6000.	34.03	34.03	34.03	34.04	34.04	34.05	34.06	34.08
8000.	33.94	33.94	33.95	33.95	33.96	33.96	33.98	33.99
10000.	33.83	33.83	33.84	33.84	33.84	33.85	33.87	33.88

Table 162. Molar volume in cm^3/g of lime, CaO, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	16.76	16.81	16.87	16.94	17.08	17.23	17.53	17.84
500.	16.75	16.81	16.86	16.93	17.07	17.22	17.52	17.83
1000.	16.74	16.80	16.86	16.92	17.06	17.21	17.51	17.82
2000.	16.73	16.78	16.84	16.90	17.04	17.19	17.49	17.81
4000.	16.69	16.74	16.80	16.87	17.01	17.16	17.46	17.77
6000.	16.66	16.71	16.77	16.84	16.98	17.12	17.43	17.74
8000.	16.63	16.68	16.74	16.81	16.95	17.09	17.40	17.71
10000.	16.60	16.65	16.71	16.78	16.92	17.06	17.37	17.68

Table 163. Molar volume in cm^3/g of wollastonite, $CaSiO_3$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	39.79	39.98	40.12	40.24	40.42	40.56	40.77	40.97
500.	39.77	39.95	40.10	40.21	40.39	40.53	40.75	40.94
1000.	39.74	39.93	40.07	40.19	40.36	40.50	40.72	40.91
2000.	39.69	39.87	40.02	40.13	40.31	40.45	40.67	40.86
4000.	39.58	39.77	39.91	40.03	40.21	40.34	40.56	40.76
6000.	39.48	39.67	39.81	39.93	40.11	40.24	40.46	40.66
8000.	39.38	39.57	39.71	39.83	40.01	40.15	40.37	40.56
10000.	39.29	39.48	39.62	39.74	39.92	40.05	40.27	40.47

Table 164. Molar volume in cm^3/g of cyclowollastonite, $CaSiO_3$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	40.16	40.20	40.25	40.31	40.45	40.60	40.92	41.24
500.	40.12	40.16	40.21	40.27	40.40	40.56	40.88	41.20
1000.	40.08	40.12	40.17	40.23	40.36	40.52	40.84	41.16
2000.	40.00	40.04	40.09	40.15	40.29	40.44	40.76	41.09
4000.	39.85	39.89	39.94	40.00	40.14	40.29	40.61	40.94
6000.	39.71	39.75	39.80	39.86	40.00	40.15	40.47	40.80
8000.	39.58	39.62	39.67	39.73	39.87	40.02	40.34	40.67
10000.	39.46	39.50	39.55	39.61	39.75	39.90	40.22	40.55

Table 165. Molar volume in cm^3/g of bicchulite, $Ca_2Al_2SiO_6(OH)_2$, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	103.55	103.93	104.31	104.68	105.43	106.19	---	---
500.	103.48	103.86	104.24	104.62	105.37	106.12	---	---
1000.	103.41	103.80	104.17	104.55	105.30	106.05	---	---
2000.	103.28	103.66	104.04	104.42	105.17	105.92	---	---
4000.	103.02	103.40	103.77	104.15	104.90	105.65	---	---
6000.	102.75	103.13	103.51	103.88	104.64	105.39	---	---
8000.	102.48	102.87	103.24	103.62	104.37	105.12	---	---
10000.	102.22	102.60	102.98	103.35	104.10	104.86	---	---

Table 166. Molar volume in cm^3/g of gehlenite, $Ca_2Al_2SiO_7$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	90.25	90.50	90.75	91.00	91.50	91.99	92.99	93.98
500.	90.23	90.48	90.73	90.98	91.48	91.97	92.97	93.96
1000.	90.21	90.46	90.71	90.96	91.46	91.95	92.95	93.94
2000.	90.17	90.42	90.67	90.92	91.41	91.91	92.91	93.90
4000.	90.08	90.34	90.59	90.84	91.33	91.83	92.82	93.82
6000.	90.00	90.26	90.50	90.75	91.25	91.75	92.74	93.74
8000.	89.92	90.17	90.42	90.67	91.17	91.67	92.66	93.66
10000.	89.84	90.09	90.34	90.59	91.09	91.58	92.58	93.57

Table 167. Molar volume in cm^3/g of prehnite, $Ca_2Al_2Si_3O_{10}(OH)_2$, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	140.43	140.96	141.47	141.98	143.00	144.03	---	---
500.	140.32	140.84	141.36	141.87	142.89	143.92	---	---
1000.	140.21	140.73	141.24	141.76	142.78	143.81	---	---
2000.	139.99	140.51	141.02	141.53	142.56	143.58	---	---
4000.	139.54	140.06	140.57	141.08	142.11	143.13	---	---
6000.	139.09	139.61	140.12	140.64	141.66	142.69	---	---
8000.	138.64	139.16	139.68	140.19	141.21	142.24	---	---
10000.	138.19	138.72	139.23	139.74	140.77	141.79	---	---

Table 168. Molar volume in cm^3/g of zoisite, $Ca_2Al_3Si_3O_{12}(OH)$, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	136.72	137.23	137.73	138.22	139.22	140.21	---	---
500.	136.64	137.14	137.64	138.14	139.14	140.13	---	---
1000.	136.55	137.06	137.56	138.06	139.05	140.05	---	---
2000.	136.39	136.90	137.39	137.89	138.89	139.88	---	---
4000.	136.06	136.57	137.06	137.56	138.56	139.55	---	---
6000.	135.73	136.23	136.73	137.23	138.23	139.22	---	---
8000.	135.40	135.90	136.40	136.90	137.89	138.89	---	---
10000.	135.06	135.57	136.07	136.57	137.56	138.56	---	---

Table 169. Molar volume in cm^3/g of alpha-Ca_2SiO_4 to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	52.30	52.49	52.68	52.87	53.25	53.63	54.39	55.15
500.	52.28	52.48	52.67	52.86	53.24	53.62	54.38	55.14
1000.	52.27	52.46	52.65	52.84	53.22	53.60	54.36	55.12
2000.	52.23	52.43	52.62	52.81	53.19	53.57	54.33	55.09
4000.	52.17	52.36	52.55	52.74	53.12	53.50	54.26	55.02
6000.	52.10	52.29	52.48	52.67	53.05	53.43	54.19	54.95
8000.	52.04	52.23	52.42	52.61	52.99	53.37	54.13	54.89
10000.	51.97	52.16	52.35	52.54	52.92	53.30	54.06	54.82

Table 170. Molar volume in cm^3/g of bredigite, Ca_2SiO_4, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	52.00	52.19	52.38	52.57	52.95	53.33	54.09	54.85
500.	51.98	52.18	52.37	52.56	52.94	53.32	54.08	54.84
1000.	51.97	52.16	52.35	52.54	52.92	53.30	54.06	54.82
2000.	51.93	52.13	52.32	52.51	52.89	53.27	54.03	54.79
4000.	51.87	52.06	52.25	52.44	52.82	53.20	53.96	54.72
6000.	51.80	52.00	52.19	52.38	52.76	53.14	53.90	54.66
8000.	51.74	51.93	52.12	52.31	52.69	53.07	53.83	54.59
10000.	51.67	51.86	52.05	52.24	52.62	53.00	53.76	54.52

Table 171. Molar volume in cm^3/g of Ca-olivine, Ca_2SiO_4, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	59.11	59.31	59.51	59.71	60.11	60.51	61.31	62.11
500.	59.09	59.30	59.50	59.70	60.10	60.50	61.30	62.10
1000.	59.07	59.28	59.48	59.68	60.08	60.48	61.28	62.08
2000.	59.04	59.24	59.44	59.64	60.04	60.44	61.24	62.04
4000.	58.97	59.17	59.37	59.57	59.97	60.37	61.17	61.97
6000.	58.90	59.10	59.30	59.50	59.90	60.30	61.10	61.90
8000.	58.83	59.03	59.23	59.43	59.83	60.23	61.03	61.83
10000.	58.76	58.96	59.16	59.36	59.76	60.16	60.96	61.76

Table 172. Molar volume in cm^3/g of larnite, Ca_2SiO_4, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	51.60	51.66	51.73	51.80	51.95	52.11	52.43	52.76
500.	51.58	51.64	51.71	51.78	51.93	52.09	52.41	52.74
1000.	51.57	51.63	51.69	51.77	51.92	52.07	52.40	52.72
2000.	51.54	51.60	51.66	51.73	51.88	52.04	52.36	52.69
4000.	51.47	51.53	51.60	51.67	51.82	51.98	52.30	52.63
6000.	51.41	51.47	51.53	51.60	51.75	51.91	52.23	52.56
8000.	51.34	51.40	51.47	51.54	51.69	51.85	52.17	52.50
10000.	51.28	51.34	51.40	51.47	51.62	51.78	52.10	52.43

Table 173. Molar volume in cm^3/g of grossular, $Ca_3Al_2Si_3O_{12}$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	125.19	125.47	125.77	126.07	126.71	127.36	128.69	130.03
500.	125.15	125.43	125.72	126.03	126.66	127.32	128.64	129.98
1000.	125.11	125.39	125.68	125.99	126.62	127.27	128.60	129.94
2000.	125.02	125.30	125.59	125.90	126.53	127.19	128.51	129.85
4000.	124.85	125.13	125.42	125.73	126.36	127.01	128.34	129.68
6000.	124.68	124.96	125.25	125.56	126.19	126.84	128.17	129.51
8000.	124.51	124.79	125.08	125.39	126.02	126.68	128.00	129.34
10000.	124.34	124.62	124.92	125.22	125.86	126.51	127.84	129.18

Table 174. Molar volume in cm^3/g of hatrurite, Ca_3SiO_5, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	72.74	72.80	72.87	72.95	73.13	73.32	73.73	74.14
500.	72.72	72.78	72.85	72.93	73.11	73.30	73.71	74.12
1000.	72.70	72.76	72.83	72.91	73.09	73.28	73.69	74.10
2000.	72.66	72.72	72.79	72.87	73.05	73.24	73.65	74.06
4000.	72.58	72.64	72.71	72.79	72.97	73.16	73.57	73.98
6000.	72.50	72.56	72.63	72.71	72.89	73.08	73.49	73.90
8000.	72.42	72.48	72.55	72.63	72.81	73.00	73.41	73.82
10000.	72.34	72.40	72.47	72.55	72.73	72.92	73.33	73.74

Table 175. Molar volume in cm^3/g of rankinite, $Ca_3Si_2O_7$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	96.50	96.62	96.73	96.86	97.11	97.37	97.91	98.45
500.	96.46	96.58	96.69	96.82	97.07	97.33	97.87	98.41
1000.	96.42	96.54	96.65	96.78	97.03	97.29	97.83	98.37
2000.	96.34	96.46	96.57	96.70	96.95	97.21	97.75	98.29
4000.	96.18	96.30	96.41	96.54	96.79	97.05	97.59	98.13
6000.	96.02	96.14	96.25	96.38	96.63	96.89	97.43	97.97
8000.	95.86	95.98	96.09	96.22	96.47	96.73	97.27	97.81
10000.	95.70	95.82	95.93	96.06	96.31	96.57	97.11	97.65

Table 176. Molar volume in cm^3/g of meionite, $Ca_4Al_6Si_6O_{24}(CO_3)$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	337.60	338.17	338.73	339.30	340.42	341.55	343.80	346.05
500.	337.38	337.95	338.51	339.08	340.20	341.33	343.58	345.84
1000.	337.16	337.73	338.30	338.86	339.99	341.11	343.36	345.62
2000.	336.72	337.30	337.86	338.42	339.55	340.68	342.93	345.18
4000.	335.85	336.42	336.99	337.55	338.68	339.80	342.05	344.31
6000.	334.98	335.55	336.11	336.68	337.80	338.93	341.18	343.43
8000.	334.10	334.68	335.24	335.80	336.93	338.06	340.31	342.56
10000.	333.23	333.80	334.37	334.93	336.06	337.18	339.44	341.69

Table 177. Molar volume in cm^3/g of wustite, $Fe_{.947}O$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	12.04	12.04	12.04	12.04	12.04	12.04	12.04	12.04
500.	12.04	12.04	12.04	12.04	12.04	12.04	12.04	12.04
1000.	12.03	12.03	12.03	12.03	12.03	12.03	12.03	12.03
2000.	12.02	12.02	12.02	12.02	12.02	12.02	12.02	12.02
4000.	12.01	12.01	12.01	12.01	12.01	12.01	12.01	12.01
6000.	11.99	11.99	11.99	11.99	11.99	11.99	11.99	11.99
8000.	11.97	11.97	11.97	11.97	11.97	11.97	11.97	11.97
10000.	11.96	11.96	11.96	11.96	11.96	11.96	11.96	11.96

Table 178. Molar volume in cm^3/g of ferrosilite, $FeSiO_3$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	32.99	33.11	33.23	33.35	33.60	33.84	34.32	34.81
500.	32.95	33.08	33.20	33.32	33.56	33.80	34.29	34.77
1000.	32.92	33.04	33.16	33.28	33.53	33.77	34.25	34.74
2000.	32.85	32.97	33.09	33.21	33.45	33.70	34.18	34.67
4000.	32.70	32.83	32.95	33.07	33.31	33.55	34.04	34.52
6000.	32.56	32.68	32.81	32.93	33.17	33.41	33.90	34.38
8000.	32.42	32.54	32.66	32.78	33.03	33.27	33.75	34.24
10000.	32.28	32.40	32.52	32.64	32.88	33.13	33.61	34.10

Table 179. Molar volume in cm^3/g of hematite, Fe_2O_3, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	30.28	30.39	30.51	30.63	30.86	31.10	31.57	32.03
500.	30.27	30.39	30.50	30.62	30.85	31.09	31.56	32.03
1000.	30.26	30.38	30.49	30.61	30.85	31.08	31.55	32.02
2000.	30.24	30.36	30.48	30.59	30.83	31.06	31.53	32.00
4000.	30.21	30.33	30.44	30.56	30.79	31.03	31.50	31.97
6000.	30.17	30.29	30.41	30.53	30.76	31.00	31.46	31.93
8000.	30.14	30.26	30.38	30.49	30.73	30.96	31.43	31.90
10000.	30.11	30.23	30.35	30.46	30.70	30.93	31.40	31.87

Table 180. Molar volume in cm^3/g of fayalite, Fe_2SiO_4, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	46.15	46.30	46.45	46.60	46.89	47.19	47.79	48.38
500.	46.13	46.28	46.43	46.58	46.88	47.17	47.77	48.36
1000.	46.11	46.26	46.41	46.56	46.86	47.16	47.75	48.35
2000.	46.08	46.23	46.38	46.53	46.82	47.12	47.72	48.31
4000.	46.01	46.16	46.31	46.46	46.75	47.05	47.65	48.24
6000.	45.94	46.09	46.24	46.39	46.68	46.98	47.58	48.17
8000.	45.87	46.02	46.17	46.32	46.61	46.91	47.51	48.10
10000.	45.80	45.95	46.10	46.25	46.54	46.84	47.44	48.03

Table 181. Molar volume in cm^3/g of magnetite, Fe_3O_4, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	44.52	44.57	44.61	44.66	44.74	44.54	44.54	44.54
500.	44.51	44.56	44.60	44.64	44.73	44.54	44.54	44.54
1000.	44.50	44.54	44.59	44.63	44.72	44.54	44.54	44.54
2000.	44.47	44.52	44.56	44.60	44.69	44.54	44.54	44.54
4000.	44.42	44.46	44.51	44.55	44.64	44.54	44.54	44.54
6000.	44.37	44.41	44.46	44.50	44.59	44.54	44.54	44.54
8000.	44.32	44.36	44.41	44.45	44.54	44.54	44.54	44.54
10000.	44.27	44.31	44.35	44.40	44.49	44.54	44.54	44.54

Table 182. Molar volume in cm^3/g of water and H_2O (real gas) to 1400 K and 10,000 bars. The tabulation is based on data cited in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1200.	1400.
1.	18.068	32460.	40854.	49132.	65601.	82035.	98458.	114876.
500.	17.690	18.744	20.732	24.520	82.569	145.900	191.664	231.875
1000.	17.358	18.350	20.034	22.762	37.363	67.766	94.032	116.557
2000.	16.809	17.714	19.044	20.904	27.152	37.597	49.725	61.299
4000.	----	16.786	17.767	18.970	22.194	26.499	31.477	36.668
6000.	----	16.114	16.906	17.813	20.035	22.782	25.863	29.086
8000.	----	15.592	16.255	16.986	18.681	20.690	22.913	25.235
10000.	----	15.170	15.732	16.342	17.704	19.274	20.997	22.802

Table 183. Molar volume in cm^3/g of magnesite, $MgCO_3$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	28.02	28.08	28.13	28.19	28.30	28.42	28.64	28.87
500.	28.00	28.06	28.11	28.17	28.28	28.40	28.62	28.85
1000.	27.98	28.04	28.10	28.15	28.27	28.38	28.61	28.83
2000.	27.95	28.00	28.06	28.12	28.23	28.34	28.57	28.80
4000.	27.87	27.93	27.99	28.04	28.16	28.27	28.50	28.72
6000.	27.80	27.86	27.92	27.97	28.09	28.20	28.43	28.65
8000.	27.73	27.79	27.84	27.90	28.01	28.13	28.35	28.58
10000.	27.66	27.72	27.77	27.83	27.94	28.06	28.28	28.51

Table 184. Molar volume in cm^3/g of periclase, MgO, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	11.24	11.29	11.33	11.37	11.45	11.54	11.70	11.87
500.	11.24	11.28	11.33	11.37	11.45	11.53	11.70	11.87
1000.	11.24	11.28	11.32	11.36	11.45	11.53	11.70	11.87
2000.	11.23	11.27	11.32	11.36	11.44	11.53	11.69	11.86
4000.	11.22	11.26	11.30	11.35	11.43	11.51	11.68	11.85
6000.	11.21	11.25	11.29	11.33	11.42	11.50	11.67	11.84
8000.	11.20	11.24	11.28	11.32	11.41	11.49	11.66	11.82
10000.	11.18	11.23	11.27	11.31	11.39	11.48	11.64	11.81

Table 185. Molar volume in cm^3/g of brucite, $Mg(OH)_2$, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	24.63	24.69	24.74	24.79	24.90	25.01	---	---
500.	24.63	24.68	24.74	24.79	24.90	25.00	---	---
1000.	24.62	24.68	24.73	24.79	24.89	25.00	---	---
2000.	24.62	24.67	24.73	24.78	24.89	24.99	---	---
4000.	24.61	24.66	24.71	24.77	24.87	24.98	---	---
6000.	24.59	24.65	24.70	24.76	24.86	24.97	---	---
8000.	24.58	24.64	24.69	24.74	24.85	24.96	---	---
10000.	24.57	24.63	24.68	24.73	24.84	24.95	---	---

Table 186. Molar volume in cm^3/g of clinoenstatite, $MgSiO_3$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	31.27	31.38	31.47	31.57	31.77	31.97	32.37	32.77
500.	31.26	31.36	31.46	31.56	31.76	31.96	32.36	32.76
1000.	31.25	31.35	31.45	31.55	31.75	31.95	32.35	32.74
2000.	31.22	31.32	31.42	31.52	31.72	31.92	32.32	32.72
4000.	31.16	31.27	31.37	31.47	31.66	31.86	32.26	32.66
6000.	31.11	31.21	31.31	31.41	31.61	31.81	32.21	32.61
8000.	31.05	31.16	31.26	31.36	31.56	31.75	32.15	32.55
10000.	31.00	31.10	31.20	31.30	31.50	31.70	32.10	32.50

Table 187. Molar volume in cm^3/g of enstatite, $MgSiO_3$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	31.35	31.42	31.50	31.58	31.77	31.97	32.38	32.80
500.	31.34	31.41	31.48	31.57	31.76	31.95	32.36	32.78
1000.	31.32	31.39	31.47	31.56	31.74	31.94	32.35	32.77
2000.	31.29	31.36	31.44	31.53	31.71	31.91	32.32	32.74
4000.	31.24	31.31	31.39	31.47	31.66	31.86	32.27	32.68
6000.	31.18	31.25	31.33	31.42	31.61	31.80	32.21	32.63
8000.	31.13	31.20	31.28	31.37	31.55	31.75	32.16	32.58
10000.	31.08	31.15	31.23	31.31	31.50	31.70	32.11	32.52

Table 188. Molar volume in cm^3/g of protoenstatite, $MgSiO_3$, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	32.34	32.43	32.53	32.62	32.80	32.99	33.36	33.73
500.	32.33	32.42	32.51	32.61	32.79	32.98	33.35	33.72
1000.	32.31	32.41	32.50	32.59	32.78	32.96	33.34	33.71
2000.	32.29	32.38	32.47	32.57	32.75	32.94	33.31	33.68
4000.	32.23	32.33	32.42	32.52	32.70	32.89	33.26	33.63
6000.	32.18	32.28	32.37	32.46	32.65	32.84	33.21	33.58
8000.	32.13	32.23	32.32	32.41	32.60	32.78	33.16	33.53
10000.	32.08	32.17	32.27	32.36	32.55	32.73	33.10	33.48

Table 189. Molar volume in cm^3/g of forsterite, Mg_2SiO_4, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	43.65	43.78	43.93	44.09	44.44	44.81	45.58	46.36
500.	43.63	43.76	43.91	44.07	44.42	44.79	45.56	46.34
1000.	43.62	43.75	43.89	44.05	44.40	44.78	45.54	46.32
2000.	43.58	43.71	43.86	44.02	44.37	44.74	45.51	46.29
4000.	43.51	43.64	43.78	43.94	44.29	44.67	45.43	46.21
6000.	43.43	43.56	43.71	43.87	44.22	44.59	45.36	46.14
8000.	43.36	43.49	43.64	43.80	44.15	44.52	45.29	46.07
10000.	43.30	43.43	43.57	43.74	44.08	44.46	45.22	46.01

Table 190. Molar volume in cm^3/g of chrysotile, $Mg_3Si_2O_5(OH)_4$, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	107.28	107.49	107.70	107.90	108.32	108.74	---	---
500.	107.15	107.37	107.57	107.78	108.20	108.62	---	---
1000.	107.03	107.25	107.45	107.66	108.08	108.50	---	---
2000.	106.80	107.01	107.22	107.43	107.84	108.26	---	---
4000.	106.35	106.56	106.77	106.97	107.39	107.81	---	---
6000.	105.92	106.13	106.34	106.55	106.96	107.38	---	---
8000.	105.52	105.73	105.94	106.14	106.56	106.98	---	---
10000.	105.13	105.35	105.56	105.76	106.18	106.60	---	---

Table 191. Molar volume in cm^3/g of talc, $Mg_3Si_4O_{10}(OH)_2$, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	135.95	136.25	136.54	136.84	137.42	138.00	---	---
500.	135.80	136.10	136.39	136.68	137.27	137.85	---	---
1000.	135.65	135.95	136.24	136.53	137.12	137.70	---	---
2000.	135.36	135.66	135.95	136.24	136.83	137.41	---	---
4000.	134.80	135.09	135.39	135.68	136.26	136.85	---	---
6000.	134.27	134.56	134.85	135.15	135.73	136.32	---	---
8000.	133.76	134.06	134.35	134.65	135.23	135.81	---	---
10000.	133.29	133.59	133.88	134.17	134.76	135.34	---	---

Table 192. Molar volume in cm^3/g of anthophyllite, $Mg_7Si_8O_{22}(OH)_2$, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	263.86	263.94	264.02	264.09	264.25	264.40	---	---
500.	263.85	263.92	264.00	264.08	264.23	264.38	---	---
1000.	263.83	263.91	263.98	264.06	264.21	264.36	---	---
2000.	263.80	263.87	263.95	264.03	264.18	264.33	---	---
4000.	263.73	263.80	263.88	263.96	264.11	264.26	---	---
6000.	263.66	263.74	263.81	263.89	264.04	264.19	---	---
8000.	263.59	263.67	263.75	263.82	263.97	264.13	---	---
10000.	263.52	263.60	263.68	263.75	263.91	264.06	---	---

Table 193. Molar volume in cm^3/g of antigorite, $Mg_{48}Si_{34}O_{85}(OH)_{62}$, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
1.	1749.15	1752.81	1756.40	1759.99	1767.17	1774.35	---	---
500.	1747.23	1750.89	1754.48	1758.07	1765.25	1772.43	---	---
1000.	1745.33	1748.99	1752.58	1756.17	1763.35	1770.53	---	---
2000.	1741.61	1745.26	1748.85	1752.44	1759.63	1766.81	---	---
4000.	1734.47	1738.13	1741.72	1745.31	1752.49	1759.68	---	---
6000.	1727.74	1731.40	1734.99	1738.58	1745.76	1752.94	---	---
8000.	1721.38	1725.04	1728.63	1732.22	1739.40	1746.58	---	---
10000.	1715.37	1719.03	1722.62	1726.21	1733.39	1740.57	---	---

Table 194. Molar volume in cm^3/g of quartz, SiO_2, to 1800 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
	alpha quartz					beta quartz		
1.	22.59	22.72	22.86	23.00	23.27	23.58	23.58	23.58
500.	22.57	22.70	22.84	22.97	23.25	23.56	23.56	23.56
1000.	22.54	22.68	22.82	22.95	23.22	23.53	23.53	23.53
2000.	22.50	22.64	22.78	22.91	23.18	23.48	23.48	23.48
4000.	22.42	22.55	22.69	22.83	23.10	23.39	23.39	23.39
6000.	22.33	22.47	22.60	22.74	23.01	23.28	23.30	23.30
8000.	22.24	22.38	22.52	22.65	22.93	23.20	23.20	23.20
10000.	22.16	22.30	22.43	22.57	22.84	23.11	23.11	23.11

Table 195. Molar volume in cm^3/g of cristobalite, SiO_2, to 1000 K and 10,000 bars. The tabulations are based on a fit of the thermophysical and thermochemical data given in Section 1.5.5.

Pressure (bars)	Temperature (K)							
	298.15	400.	500.	600.	800.	1000.	1400.	1800.
	alpha cristobalite			beta cristobalite				
1.	25.81	26.07	26.33	27.36	27.40	27.44	27.53	27.61
500.	25.77	26.04	26.29	27.33	27.37	27.41	27.50	27.58
1000.	25.74	26.00	26.26	27.29	27.34	27.38	27.46	27.55
2000.	25.68	25.94	26.20	27.23	27.27	27.31	27.40	27.48
4000.	25.55	25.81	26.07	26.33	27.14	27.18	27.27	27.35
6000.	25.42	25.68	25.94	26.20	27.01	27.05	27.14	27.22
8000.	25.29	25.55	25.81	26.07	26.58	26.93	27.01	27.10
10000.	25.16	25.42	25.68	25.94	26.45	26.80	26.88	26.97

1.5.5. Summaries of Data Sources, Standard State Properties, and Fitted Functions Describing Mineral Thermodynamics and Thermophysical Properties

The sources of data used for the evaluation of the properties, both thermophysical and thermochemical, are given in this section. They are arranged by chemical formula in the same order as they appear in section 1.5.4.

Tables 10 and 11 list the table numbers for thermophysical, thermochemical, and volumetric properties of these phases.

The constants that are to be used in the algebraic functions given in section 1.5.3 are given below in section 1.5.5.49.

1.5.5.1. Al, aluminum (formula weight = 28.892 g/mol)

The properties of aluminum were taken from the JANAF thermochemical data[a]. The molar volume of aluminum was not needed in this study and therefore was not evaluated.

1.5.5.2. AlOOH (formula weight = 59.989 g/mol)

1.5.5.2.1. Boehmite

Tables 196 and 197 contain the data used in the final evaluation. All other data, though cited in the reference list, were dropped before the final evaluation.

Shomate and Cook (1946) measured the heat content of a boehmite sample between 298 and 520 K. However, the data do not smoothly connect with the low-temperature data and appear to be too low. It is probable that there was loss of H_2O from the sample without

[a]JANAF Thermochemical Tables, looseleaf pages for 1979 issued by Dow Chemical Company, 1707 Building, Midland, Michigan.

Table 196. Sources of thermophysical data for boehmite, AlOOH.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	0.00
Shomate and Cook, 1946	heat capacity	isotherm. cal.	10	206-296	1.01	0.01±0.20
Haas and others, 1981	heat capacity	estimate	7	298-600	1.01	0.10±0.16
Robie and others, 1979	entropy	compilation	1	298	1.01	0.01

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 197. Sources of thermochemical data for boehmite, AlOOH.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
AA	Hemley and others, 1980	H_4SiO_4 concentration	3	473-523	1.0	71.058±1.042	-990.230
AV	Chang, 1981	Differential Solubility in Water	1	333	0.001	16.758±0.359	-992.066
	This Study						-990.654

Reactions:

AA $2\ AlOOH[boehmite] + 2\ H_4SiO_4[aqueous,\ 1\ kb] = Al_2Si_2O_5(OH)_4[kaolinite] + 3\ H_2O[g]$

AV $Al(OH)_3[gibbsite] = AlOOH[boehmite] + H_2O(l)$

correction for the change in weight and phase content. Mukaibo and others (1969) measured the heat capacity of an impure boehmite between 3.2 and 585 K. The sample contained about 1 percent excess H_2O and had a heat capacity about 1.3 percent lower than the estimated values of Haas and others (1981). The excess H_2O was probably present as admixed gibbsite. The lower heat capacity is consistent with such a hypothesis.

Hemley and others (1980) measured the concentration of silicic acid coexisting with the mineral pair boehmite + kaolinite. During the previous effort (Haas and others, 1981), it was recognized that the experiments lead to a possible inversion of diaspore to boehmite about 570 to 600 K. Discussions at that time and since then with J.J. Hemley indicate that the inversion may exist. Acting upon the suggestion of Hemley, in this evaluation we have used the data that would make boehmite the least stable, that is, we used the three points that had the lowest silicic acid concentration for the temperature of observation. The inversion as derived from this evaluation is calculated to be 583.55 K at 1.01 bars.

1.5.5.2.2. Diaspore

Tables 198 and 199 contain the data used in the final evaluation of the properties of diaspore. Other data, though cited in the reference list, were dropped before the final evaluation.

The heat capacity of diaspore is based on the recent work of Perkins and others (1979). The earlier work by King and Weller (1961a) is in reasonable agreement though it averages slightly lower.

Table 198. Sources of thermophysical data for diaspore, AlOOH.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	0.00
King and Weller, 1961a	heat capacity	isotherm. cal.	10	206-296	1.01	-0.68±0.22
Perkins and others, 1979	heat capacity	adiab. cal.	15	204-345	1.01	0.23±0.22
Perkins and others, 1979	heat capacity	d.s.c.	19	340-509	1.01	-0.61±1.03
Perkins and others, 1979	entropy	adiab. cal.	1	298	1.01	-0.003

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 199. Sources of thermochemical data for diaspore, AlOOH.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
AB	Hemley and others, 1980	H_4SiO_4 concentration	6	473-573	1.0	88.372±0.414	-1000.151
AC	Hemley and others, 1980	H_4SiO_4 concentration	3	523-573	2.0	239.616±1.809	-1001.264
AC	Hemley and others, 1980	H_4SiO_4 concentration	1	598	1.0	295.910	-999.650
AD	Hemley and others, 1980	H_4SiO_4 concentration	2	623-663	1.0	151.551±0.163	-999.248
AZ	Haas and Holdaway, 1973	Gas-medium Pressure Apparatus	4 pr	618-722	2.4-7.0	306.234±3.143	-999.594
BK	Haas, 1972	Gas-medium Pressure Apparatus	5 pr	662-741	1.75-7.0	81.731±0.686	-1000.235
	This Study						-999.944

Reactions:

AB 2 AlOOH[diaspore] + 2 H_4SiO_4[aqueous, 1 kb] = $Al_2Si_2O_5(OH)_4$[kaolinite] + 3 H_2O[g]

AC 2 AlOOH[diaspore] + 4 H_4SiO_4[aqueous, 1 or 2 kb] = $Al_2Si_4O_{10}(OH)_2$[pyrophyllite] + 8 H_2O[g]

AD 2 AlOOH[diaspore] + H_4SiO_4[aqueous, 1 kb] = Al_2SiO_5[andalusite] + 3 H_2O[g]

AZ 6 AlOOH[diaspore] + $Al_2Si_4O_{10}(OH)_2$[pyrophyllite] = 4 Al_2SiO_5[andalusite] + 4 H_2O[g]

BK 2 AlOOH[diaspore] = Al_2O_3[corundum] + H_2O[g]

The heat capacity was also measured by Mukaibo and others (1969) on an impure, H_2O-deficient sample to near 600 K. These data are slightly higher than those of Perkins and others. Mukaibo and others did not make composition corrections on their data, and this departure would be expected if a less-hydrous phase such as corundum were present.

The phase equilibria studies of Hemley and others (1980), Haas (1972), and Haas and Holdaway (1973) are in good agreement. Depending upon the work by J.J. Hemley currently in progress, the decomposition reaction of diaspore to corundum and H_2O[gas] may be metastable.

1.5.5.3. $Al(OH)_3$, gibbsite (formula weight = 78.004 g/mol)

The data used to evaluate the properties of gibbsite are given in tables 200 and 201.

In addition to these data, Hemingway and others (1977) measured the enthalpy of the reaction:

$$Al[c] + 3\ H_2O[liq] = Al(OH)_3[gibbsite] + 1.5\ H_2O[gas]$$

They obtained an enthalpy, when reduced to 298.15 K, of -435.957 ± 3.173 kJ/mol as compared to -437.209 kJ/mol calculated from the tabulated properties. The departure is 1.252 kJ/mol. These results are an independent check on the enthalpy of formation recommended by the CODATA Task Group on Key Values for Thermodynamics (1978) and used in preparing the JANAF Thermochemical Tables[a].

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[a]JANAF Thermochemical Tables, looseleaf pages for 1979 issued by Dow Chemical Company, 1707 Building, Midland, Michigan.

Table 200. Sources of thermophysical data for gibbsite, $Al(OH)_3$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	0.0
Megaw, 1933	expansivity	dilatometry	1	298	1.01	0.0
Hemingway and others, 1977	heat capacity	adiab. cal. and d.s.c.	23	200-479	1.01	-0.03±0.29
Hemingway and others, 1977	entropy	adiab. cal.	1	298	1.01	0.0

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 201. Sources of thermochemical data for gibbsite, $Al(OH)_3$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
AV	Chang, 1981	Differential Solubility in Water	1	333	0.001	16.758±0.359	-1296.045
BO	Kracek and Neuvonen, 1952	Solution calorimetry, HF acid	1	347	0.001	43.470±0.581	-1293.584
BR	Barany and Kelley, 1961	Solution calorimetry, HF acid	6	347	0.001	7.570±0.383	-1294.567
BS	Barany and Kelley, 1961	Solution calorimetry, HF acid	6	347	0.001	-9.873±0.342	-1294.567
BT	Barany and Kelley, 1961	Solution calorimetry, HF acid	15	347	0.001	8.830±0.355	-1294.621
	This Study						-1294.633

Reactions:

AV $Al(OH)_3$[gibbsite] = AlOOH[boehmite] + H_2O(l)

BO $CaAl_2Si_2O_8$[anorthite] + 3 H_2O[l] = CaO[lime] + 2 $Al(OH)_2$[gibbsite] + 2 SiO_2[quartz, alpha]

BR $Al_2Si_2O_5(OH)_4$[dickite] + H_2O[l] = 2 $Al(OH)_3$[gibbsite] + 2 SiO_2[quartz, alpha]

BS $Al_2Si_2O_5(OH)_4$[halloysite] + H_2O[l] = 2 $Al(OH)_3$[gibbsite] + 2 SiO_2[quartz, alpha]

BT $Al_2Si_2O_5(OH)_4$[kaolinite] + H_2O[l] = 2 $Al(OH)_3$[gibbsite] + 2 SiO_2[quartz, alpha]

1.5.5.4. Al_2O_3, corundum (formula weight = 101.962 g/mol)

The properties of corundum, with the exception of molar volume, were taken from the JANAF Thermochemical Tables[a]. Table 202 contains the sources of data for the molar volume as a function of temperature and pressure.

1.5.5.5. Al_2SiO_5 (formula weight = 162.047 g/mol)

The stable polymorphs of Al_2SiO_5 have calculated inversions at 1.01 bars as follows:

Inversion	Temperature
kyanite = andalusite	408.45 K
andalusite = sillimanite	942.45 K

The data used to establish these reactions as well as the phase equilibria with other minerals are cited below.

1.5.5.5.1. Andalusite

Tables 203 and 204 contain the data used in the final evaluation. All other data, though cited in the reference list, were dropped before the final evaluation.

The molar volumes as measured by Winter and Ghose (1979) are smaller than those measured earlier by Skinner and others (1961). The recent data of Schneider (1979) are intermediate between the two data sets. Because of the scatter, all sets are included in the

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[a]JANAF Thermochemical Tables, looseleaf pages for 1979 issued by Dow Chemical Company, 1707 Building, Midland, Michigan.

Table 202. Sources of volumetric data for corundum, Al_2O_3.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Schauer, 1965	volume	X-ray	13	300-1470	1.01	-0.01±0.13
Skinner, 1966	volume	X-ray	8	298-1473	1.01	-0.03±0.06
d'Amour and others, 1978	volume	X-ray	7	298	1.01-90000	0.17±0.19
Finger and Hazen, 1978	volume	X-ray	7	296	1.01-80000	-0.11±0.29

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 203. Sources of thermophysical data for andalusite, Al_2SiO_5.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and Hemingway, 1982(unpub.)	compressibility	estimate		298	1.01	36.56
Ralph and others, 1981	volume	X-ray	4	298	1.01-37000	-0.02±0.07
Schneider, 1979	volume	X-ray	2	473-1273	1.01	0.04±0.05
Skinner and others, 1961	volume	X-ray	11	290-1281	1.01	0.15±0.23
Winter and Ghose, 1979	volume	X-ray	5	298-1273	1.01	-0.20±0.18
Brace and others, 1969	compressibility	dilatometry	10	298	1000-40000	3.64±3.86
Robie and Hemingway, 1982(unpub.)	heat capacity	adiab. cal.	29	226-377	1.01	0.02±0.16
Pankratz and Kelley, 1964b	heat content	drop cal.	13	397-1601	1.01	-0.14±0.31
Robie and Hemingway, 1982(unpub.)	entropy	adiab. cal.	1	298	1.01	-0.11

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 204. Sources of thermochemical data for andalusite, Al_2SiO_5.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
AD	Hemley and others, 1980	H_4SiO_4 concentration	2	623-663	1.0	151.551±0.163	-2591.234
AK	Hemley and others, 1980	H_4SiO_4 concentration	3	623-633	2.0	105.020±2.107	-2593.264
AK	Hemley and others, 1980	H_4SiO_4 concentration	8	613-673	1.0	143.886±0.594	-2595.079
AL	Holdaway, 1971	Gas-medium Pressure Apparatus	2 pr	764-917	1.8-3.6	3.833±0.102	-2592.516
AL	Weill, 1966	Differential Solubility in Melt	2	1073-1283	0.001	4.466±0.333	-2593.369
AM	Storre and Nitsch, 1974	Gas- and Solid-medium Pressure Apparatus	2 pr	788-833	4.0-5.0	-88.085±1.706	-2592.287
AX	Holdaway, 1971	Gas-medium Pressure Apparatus	3 pr	650-858	2.4-4.8	3.994±0.205	-2592.352
AX	Newton, 1966a	Gas-medium Pressure Apparatus	7	973-1123	6.1-7.4	3.637±0.226	-2592.707
AZ	Haas and Holdaway, 1973	Gas-medium Pressure Apparatus	4 pr	618-722	2.4-7.0	306.234±3.143	-2592.105
BA	Haas and Holdaway, 1973	Gas-medium Pressure Apparatus	4 pr	643-737	2.4-7.0	75.319±0.620	-2593.155
BM	Hemley and others, 1980	H_4SiO_4 concentration	4	723-773	2.0	53.445±0.276	-2593.465
BM	Hemley and others, 1980	H_4SiO_4 concentration	6	723-753	1.0	67.312±0.156	-2593.158
AX	Anderson and others, 1977	Solution calorimetry, borate salt	1	970	0.001	5.720±0.685	-2591.474
	This Study						-2592.626

Reactions:

AD $2\ AlOOH[diaspore] + H_4SiO_4[aqueous,\ 1\ kb] = Al_2SiO_5[andalusite] + 3\ H_2O[g]$

AK $Al_2SiO_5[andalusite] + 3\ H_4SiO_4[aqueous,\ 1\ or\ 2\ kb] + H_2O[g] = Al_2Si_4O_{10}(OH)_2[pyrophyllite] + 5\ H_2O[g]$

AL $Al_2SiO_5[andalusite] = Al_2SiO_5[sillimanite]$

AM $Al_2SiO_5[andalusite] + CaAl_2Si_2O_8[anorthite] + H_2O[g] = CaAl_4Si_2O_{10}(OH)_2[margarite] + SiO_2[quartz,\ alpha]$

AX $Al_2SiO_5[kyanite] = Al_2SiO_5[andalusite]$

AZ $6\ AlOOH[diaspore] + Al_2Si_4O_{10}(OH)_2[pyrophyllite] = 4\ Al_2SiO_5[andalusite] + 4\ H_2O[g]$

BA $Al_2Si_4O_{10}(OH)_2[pyrophyllite] = Al_2SiO_5[andalusite] + 3\ SiO_2[quartz,\ alpha] + H_2O[g]$

BM $Al_2SiO_5[andalusite] + 2\ H_2O[g] = Al_2O_3[corundum] + H_4SiO_4[aqueous,\ 1\ or\ 2\ kb]$

evaluated data set and the results are most consistent with Schneider's data, as would be expected.

There is disagreement between the changes in the molar volumes as measured by Ralph and others (1981) and the compressibility as calculated from the elastic constants by Robie and Hemingway (1982, unpub.). However, the mechanically measured compressibilities obtained by Brace and others (1969) are in reasonable agreement with the measured volumes. All three sets were included. The evaluation rejected the calculated compressibility and favored the other sets.

The earlier low-temperature heat capacities of Todd (1950) have been replaced by new measurements of better samples by Robie and Hemingway (in review). The high-temperature heat capacities were obtained from the work of Pankratz and Kelley (1964b).

The data relating the stability of andalusite to other minerals as given in table 204 are reasonably consistent. The major exception is the experiments of Hemley and others (1980) for the concentration of aqueous silicic acid coexisting with pyrophyllite and andalusite at 1 kb. The results for the same mineral pair at 2 kb are in good agreement with the results of Haas and Holdaway (1973) for the breakdown of pyrophyllite.

1.5.5.5.2. Kyanite

The data used in the final evaluation are given on tables 205 and 206. Other data, though cited in the reference list, were dropped before the final evaluation.

Table 205. Sources of thermophysical data for kyanite, Al_2SiO_5.

Source	Data type	Method	Number of points	Range		
				Temperature (K)	Pressure (bars)	Percent error[a]
Skinner and others, 1961	volume	X-ray	8	298-1328	1.01	-0.05±0.05
Winter and Ghose, 1979	volume	X-ray	4	298-1073	1.01	0.02±0.04
Bruce and others, 1969	volume diff.	dilatometry	10	298	1000-40000	-0.27±4.55
Robie and Hemingway, 1982(unpub.)	heat capacity	adiab. cal.	31	225-370	1.01	0.00±0.11
Pankratz and Kelley, 1964b	heat content	drop cal.	12	390-1503	1.01	0.12±0.25
Robie and Hemingway, 1982(unpub.)	entropy	adiab. cal.	1	298	1.01	-0.13

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 206. Sources of thermochemical data for kyanite, Al_2SiO_5.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H_f°(298.15 K) Third Law, kJ	H_f°(298.15 K) kJ/mol
AX	Holdaway, 1971	Gas-medium Pressure Apparatus	3 pr	650-858	2.4-4.8	3.994±0.205	-2598.072
AX	Newton, 1966a	Gas-medium Pressure Apparatus	7	973-1123	6.1-7.4	3.637±0.226	-2598.427
AY	Storre and Nitsch, 1974	Gas- and Solid-medium Pressure Apparatus	3 pr	803-933	5.0-9.0	-86.359±0.132	-2600.000
BB	Weill, 1966	Differential Solubility in Melt	1	1073	0.001	-7.830	-2598.733
AX	Anderson and others, 1977	Solution calorimetry, borate salt	1	970	0.001	5.720±0.685	-2597.194
BB	Anderson and Kleppa, 1969	Solution calorimetry, borate salt	1	970	0.001	8.839±0.312	-2598.951
BU	Anderson and Kleppa, 1969	Solution calorimetry, borate salt	1	970	0.001	3.793±1.296	-2596.853
	This Study						-2598.346

Reactions:

AX Al_2SiO_5[kyanite] = Al_2SiO_5[andalusite]

AY $CaAl_2Si_2O_8$[anorthite] + Al_2SiO_5[kyanite] + H_2O[g] = $CaAl_4Si_2O_{10}(OH)_2$[margarite] + SiO_2[quartz, alpha]

BB Al_2SiO_5[sillimanite] = Al_2SiO_5[kyanite]

BU Al_2SiO_5[kyanite] + $CaSiO_3$[wollastonite] = $CaAl_2Si_2O_8$[anorthite]

The thermochemical data are based primarily on the reversed equilibria among the polymorphs kyanite, sillimanite, and andalusite by Newton (1966a), Holdaway (1971), and Weill (1966).

There remains an inconsistency between the studies of the molar volume by Winter and Ghose (1979) and by Skinner and others (1961). As stated in the discussion for andalusite, the data necessary to discriminate between the sets are not available.

1.5.5.5.3. Sillimanite

Tables 207 and 208 contain the sources of data used in the final evaluation. As with kyanite and andalusite, there is a disagreement between the molar volume studies of Skinner and others (1961) and of Winter and Ghose (1979) and between the compressibility calculated from elastic constants (Robie and Hemingway, 1982, unpub.) and the compressibility derived from dilatometry (Brace and others, 1969). As with the andalusite, all data were used in the final evaluation.

The results of the evaluation of the thermochemical data agree best with the andalusite-sillimanite equilibrium study by Holdaway (1971). The departures from the other studies are within the precision of the observations.

1.5.5.6. $Al_2Si_2O_5(OH)_4$ (formula weight = 258.162 g/mol)

Kaolinite is the stable polymorph in this system at 1.01 bars. The phases dickite and halloysite are metastable to kaolinite. Tables for kaolinite are given in lieu of a reference table for the system.

Table 207. Sources of thermophysical data for sillimanite, Al_2SiO_5.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and Hemingway, 1982(unpub.)	compressibility	calc. from elas. const.	1	298	1.01	34.32
Skinner and others, 1961	volume	X-ray	11	293-1328	1.01	-0.16±0.16
Brace and others, 1969	volume diff.	dilatometry	10	298	1000-40000	-0.42±1.05
Winter and Ghose, 1979	volume	X-ray	5	298-1273	1.01	0.04±0.05
Robie and Hemingway, 1982(unpub.)	heat capacity	adiab. cal.	34	217-378	1.01	-0.06±0.15
Pankratz and Kelley, 1964b	heat content	drop cal.	13	401-1496	1.01	0.04±1.18
Robie and Hemingway, 1982(unpub.)	entropy	adiab. cal.	1	298	1.01	0.22

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 208. Sources of thermochemical data for sillimanite, Al_2SiO_5.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H_r°(298.15 K) Third Law, kJ	H_f°(298.15 K) kJ/mol
AL	Holdaway, 1971	Gas-medium Pressure Apparatus	2 pr	764-917	1.8-3.6	3.833±0.102	-2588.792
AL	Weill, 1966	Differential Solubility in Melt	2	1073-1283	0.001	4.466±0.333	-2589.645
BB	Weill, 1966	Differential Solubility in Melt	1	1073	0.001	-7.830	-2589.289
BB	Anderson and Kleppa, 1969	Solution calorimetry, borate salt	1	970	0.001	8.839±0.312	-2589.507
	This Study						-2588.902

Reactions:

AL Al_2SiO_5[andalusite] = Al_2SiO_5[sillimanite]

BB Al_2SiO_5[sillimanite] = Al_2SiO_5[kyanite]

1.5.5.6.1. Kaolinite

The data used in the final evaluation are given in tables 209 and 210. All other data, though cited in the reference list, were deleted prior to the final evaluation. All the data in table 210 are in reasonable agreement. However, as cited in the text, the phase equilibrium study of Thompson (1970) was not used in the final evaluation because it is believed that equilibrium of stable phases was not observed.

1.5.5.6.2. Dickite

Tables 211 and 212 contain the data for dickite used in the final evaluation. The thermochemical properties are based on the measured heats of solution of six dickite samples in HF acid as compared with the stoichiometrically equivalent solution of gibbsite (Barany and Kelley, 1961), water (Barany, 1963), and quartz (Bennington and others, 1978) also in HF acid.

1.5.5.6.3. Halloysite

Tables 213 and 214 contain the data for halloysite used in the final evaluation. The thermochemical properties are based on the heat of solution of six halloysite samples in HF acid as compared with the stoichiometrically equivalent solution of quartz (Bennington and others, 1978), gibbsite (Barany and Kelley, 1961), and water (Barany, 1963) also in HF acid.

Table 209. Sources of thermophysical data for kaolinite, $Al_2Si_2O_5(OH)_4$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	0.04
Hemingway and others, 1978	heat capacity	d.s.c.	14	345-500	1.01	0.38±0.45
King and Weller, 1961a	heat capacity	isotherm. cal.	10	206-296	1.01	0.03±0.20
King and Weller, 1961a	entropy	isotherm. cal.	1	298	1.01	-0.17

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 210. Sources of thermochemical data for kaolinite, $Al_2Si_2O_5(OH)_4$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
AA	Hemley and others, 1980	H_4SiO_4 concentration	3	473-523	1.0	71.058±1.042	-4132.767
AB	Hemley and others, 1980	H_4SiO_4 concentration	6	473-573	1.0	88.372±0.414	-4134.030
AW	Hemley and others, 1980	H_4SiO_4 concentration	3	523-573	2.0	181.898±1.307	-4132.309
AW	Hemley and others, 1980	H_4SiO_4 concentration	7	473-573	1.0	207.739±0.178	-4133.588
BT	Barany and Kelley, 1961	Solution calorimetry, HF acid	15	347	0.001	8.830±0.355	-4133.604
	This Study						-4133.616

Reactions:

AA $2\ AlOOH[boehmite] + 2\ H_4SiO_4[aqueous,\ 1\ kb] = Al_2Si_2O_5(OH)_4[kaolinite] + 3\ H_2O[g]$

AB $2\ AlOOH[diaspore] + 2\ H_4SiO_4[aqueous,\ 1\ kb] = Al_2Si_2O_5(OH)_4[kaolinite] + 3\ H_2O[g]$

AW $Al_2Si_2O_5(OH)_4[kaolinite] + 2\ H_4SiO_4[aqueous,\ 1\ or\ 2\ kb] = Al_2Si_4O_{10}(OH)_2[pyrophyllite] + 5\ H_2O[g]$

BT $Al_2Si_2O_5(OH)_4[kaolinite] + H_2O[l] = 2\ Al(OH)_3[gibbsite] + 2\ SiO_2[quartz,\ alpha]$

Table 211. Sources of thermophysical data for dickite, $Al_2Si_2O_5(OH)_4$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	0.0
Haas and others, 1981	heat capacity	estimate	14	340-500	1.01	0.38±0.45
King and Weller, 1961a	heat capacity	isotherm. cal.	10	206-296	1.01	-0.02±0.11
King and Weller, 1961a	entropy	isotherm. cal.	1	298	1.01	0.0

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 212. Sources of thermochemical data for dickite, $Al_2Si_2O_5(OH)_4$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H_r°(298.15 K) Third Law, kJ	H_f°(298.15 K) kJ/mol
BR	Barany and Kelley, 1961	Solution calorimetry, HF acid	6	347	0.001	7.570±0.383	-4132.236
	This study						-4132.302

Reactions:

BR $Al_2Si_2O_5(OH)_4$[dickite] + H_2O[l] = 2 $Al(OH)_3$[gibbsite] + 2 SiO_2[quartz, alpha]

Table 213. Sources of thermophysical data for halloysite, $Al_2Si_2O_5(OH)_4$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	0.0
Haas and others, 1981	heat capacity	estimate	14	340-500	1.01	-0.10±0.37
King and Weller, 1961a	heat capacity	isotherm. cal.	10	207-296	1.01	0.02±0.21
King and Weller, 1961a	entropy	isotherm. cal.	1	298	1.01	0.0

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 214. Sources of thermochemical data for halloysite, $Al_2Si_2O_5(OH)_4$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Pressure (kb)	H_r°(298.15 K) Third Law, kJ	H_f°(298.15 K) kJ/mol
BS	Barany and Kelley, 1961	Solution calorimetry, HF acid	6	347	0.001	-9.873±0.342	-4114.793
	This study						-4114.854

Reactions:

BS $Al_2Si_2O_5(OH)_4$[halloysite] + H_2O[l] = 2 $Al(OH)_3$[gibbsite] + 2 SiO_2[quartz, alpha]

1.5.5.7. $Al_2Si_4O_{10}(OH)_2$, pyrophyllite (formula weight = 360.317 g/mol)

Tables 215 and 216 contain the sources of data used in the final evaluation of the properties of pyrophyllite. Other data, though cited in the reference list, were deleted prior to the final evaluation. All the data used in the final evaluation are in acceptable internal agreement.

1.5.5.8. C, graphite (formula weight = 12.011 g/mol)

The properties of graphite were taken from the JANAF Thermochemical Tables[a]. The molar volume of graphite was not needed in this study and therefore not evaluated.

1.5.5.9. CO, carbon monoxide (ideal gas, formula weight = 28.010 g/mol)

The properties of carbon monoxide ideal gas was taken from the JANAF Thermochemical Tables (Stull and Prophet, 1971). The molar volume was not needed for this study and therefore not evaluated.

1.5.5.10. CO_2, carbon dioxide (ideal gas, formula weight = 44.010 g/mol)

The thermodynamic properties of the ideal gas at 1.01 bars were taken from the JANAF Thermochemical Tables (Stull and Prophet, 1971). The corrections for the real gas as a function of pressure at constant temperature were taken from the work of Jacobs and Kerrick (1981).

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[a]JANAF Thermochemical Tables, looseleaf pages for 1978 issued by Dow Chemical Company, 1707 Building, Midland, Michigan.

Table 215. Sources of thermophysical data for pyrophyllite, $Al_2Si_4O_{10}(OH)_2$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Taylor and Bell, 1970	volume	X-ray	7	295-675	1.01	-0.02±0.04
Robie and others, 1976	heat capacity	adiab. cal.	20	200-370	1.01	0.03±0.10
Krupka and others, 1979	heat capacity	d.s.c.	48	335-679	1.01	-0.30±0.51
Robie and others, 1976	entropy	adiab. cal.	1	298	1.01	0.029

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 216. Sources of thermochemical data for pyrophyllite, $Al_2Si_4O_{10}(OH)_2$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_f(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
AC	Hemley and others, 1980	H_4SiO_4 concentration	3	523-573	2.0	239.616±1.809	-5644.960
AC	Hemley and others, 1980	H_4SiO_4 concentration	1	598	1.0	295.910	-5641.731
AK	Hemley and others, 1980	H_4SiO_4 concentration	3	623-633	2.0	105.020±2.107	-5642.957
AK	Hemley and others, 1980	H_4SiO_4 concentration	8	613-673	1.0	143.886±0.594	-5644.772
AW	Hemley and others, 1980	H_4SiO_4 concentration	3	523-573	2.0	181.898±1.307	-5641.012
AW	Hemley and others, 1980	H_4SiO_4 concentration	7	473-573	1.0	207.739±0.178	-5642.291
AZ	Haas and Holdaway, 1973	Gas-medium Pressure Apparatus	4 pr	618-722	2.4-7.0	306.234±3.143	-5640.221
BA	Haas and Holdaway, 1973	Gas-medium Pressure Apparatus	4 pr	643-737	2.4-7.0	75.319±0.620	-5642.848
	This Study						-5642.319

Reactions:

AC $2\ AlOOH[diaspore] + 4\ H_4SiO_4[aqueous,\ 1\ or\ 2\ kb] = Al_2Si_4O_{10}(OH)_2[pyrophyllite] + 8\ H_2O[g]$

AK $Al_2SiO_5[andalusite] + 3\ H_4SiO_4[aqueous,\ 1\ or\ 2\ kb] + H_2O[g] = Al_2Si_4O_{10}(OH)_2[pyrophyllite] + 5\ H_2O[g]$

AW $Al_2Si_2O_5(OH)_4[kaolinite] + 2\ H_4SiO_4[aqueous,\ 1\ or\ 2\ kb] = Al_2Si_4O_{10}(OH)_2[pyrophyllite] + 5\ H_2O[g]$

AZ $6\ AlOOH[diaspore] + Al_2Si_4O_{10}(OH)_2[pyrophyllite] = 4\ Al_2SiO_5[andalusite] + 4\ H_2O[g]$

BA $Al_2Si_4O_{10}(OH)_2[pyrophyllite] = Al_2SiO_5[andalusite] + 3\ SiO_2[quartz,\ alpha] + H_2O[g]$

1.5.5.11. Ca, calcium (formula weight = 40.08 g/mol)

The heat capacity, heat content, and inversion-related data were taken from the compilation of Hultgren and others (1973). The entropy at 298.15 K for calcium was taken from the CODATA Task Group (1978). The volumetric data for calcium were not needed in this study and, therefore, were not evaluated.

1.5.5.12. $CaAl_2SiO_6$, Ca-Al clinopyroxene (formula weight = 218.085 g/mol)

Tables 217 and 218 contain the data used in the final evaluation. All other data, though cited in the reference list, were dropped before the final evaluation.

In addition to the thermochemical data cited on table 218, Hays (1966) observed four reversals for reaction AI. His results lead to an enthalpy of formation from the elements at 298.15 K of -3297.035 kJ/mol, a value 1.6 kJ/mol less stable than obtained through the weighted refinement. Hays used a solid-medium piston cylinder apparatus in his experiments without a pressure correction. The recent work by Gasparik (1981) used a salt medium. The pressure correction is negligible and the data are consistent with the other data in the evaluation.

1.5.5.13. $CaAl_2Si_2O_8$, anorthite (formula weight = 278.209 g/mol)

Tables 219 and 220 contain the data used in the final evaluation. All other data, though cited in the reference list, were dropped before the final evaluation.

Table 217. Sources of thermophysical data for Ca-Al clinopyroxene, $CaAl_2SiO_6$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Haselton, H.T., Jr., 1982(unpub.)	volume	X-ray	7	298-1473	1.01	0.00±0.09
Thompson and others, 1978	heat capacity	d.s.c.	16	298-1000	1.01	-0.01±0.13

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 218. Sources of thermochemical data for Ca-Al clinopyroxene, $CaAl_2SiO_6$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
Al	Gasparik, 1981	Solid-medium Pressure Apparatus	3 pr	1463-1673	10.75-23.5	-94.622±2.588	-3298.650
AO	Hays, 1966	Solid-medium Pressure Apparatus	4 pr	1473-1673	11.0-14.6	-6.335±1.964	-3298.564
BP	Charlu and others, 1978	Solution calorimetry, borate salt	1	970	0.001	67.438±1.972	-3302.204
	This Study						-3298.625

Reactions:

Al $3\ CaAl_2SiO_6$[Ca-Al clinopyroxene] = $Ca_3Al_2Si_3O_{12}$[grossular] + $2\ Al_2O_3$[corundum]

AO $CaAl_2Si_2O_8$[anorthite] + $Ca_2Al_2SiO_7$[gehlenite] + Al_2O_3[corundum] = $3\ CaAl_2SiO_6$[Ca-Al clinopyroxene]

BP $Ca_3Al_2Si_3O_{12}$[grossular] = $CaAl_2SiO_6$[Ca-Al clinopyroxene] + $2\ CaSiO_3$[wollastonite]

Table 219. Sources of thermophysical data for anorthite, $CaAl_2Si_2O_8$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Kozu and Ueda, 1933	volume diff.	dilatometry	24	323-1273	1.01	8.56±10.28
Birch, 1966	volume	compilation	5	298	1.01-40000	0.01±0.03
Grundy and Brown, 1974	volume	X-ray	8	298-1123	1.01	0.00±0.10
Hemingway and others, 1981	heat capacity	d.s.c.	95	349-986	1.01	-0.09±0.46
Robie and others, 1978	heat capacity	adiab. cal.	49	202-381	1.01	0.01±0.18
White, 1919	heat content	drop cal.	9	1173-1673	1.01	-0.02±0.24
Ferrier, 1969	heat content	drop cal.	6	1300-1800	1.01	-0.08±0.23
Robie and others, 1978	entropy	adiab. cal.	1	298	1.01	0.01

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 220. Sources of thermochemical data for anorthite, $CaAl_2Si_2O_8$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
AE	Newton, 1965	Gas- and Solid-medium Pressure Apparatus	6 pr	843-1113	2.0-6.8	-304.099±2.670	-4231.021
AE	Boettcher, 1970	Gas-medium Pressure Apparatus	1 pr	898-928	3.0	-305.304±3.803	-4231.222
AF	Hays, 1966	Solid-medium Pressure Apparatus	2 pr	1473-1523	7.5-11.0	-157.994±6.068	-4228.743
AF	Huckenholz, 1974	Unspecified	6 pr	1125-1423	0.2-7.5	-158.840±1.799	-4229.589
AF	Shmulovich, 1974	Gas-medium Pressure Apparatus	1 pr	1133-1153	0.506	-159.474±1.420	-4231.171
AG	Boettcher, 1970	Gas-medium Pressure Apparatus	2 pr	893-1053	3.0-5.9	-50.204±1.453	-4230.713
AG	Newton, 1966b	Gas-medium Pressure Apparatus	2 pr	803-923	1.1-2.0	-51.867±3.013	-4232.951
AG	Newton, 1966b	Gas-medium Pressure Apparatus	2 pr	973-1023	4.7-5.7	-48.971±1.851	-4229.481
AG	Huckenholz, 1974	Unspecified	1 pr	848-858	2.0	-49.455±0.327	-4230.540
AG	Huckenholz, 1974	Unspecified	2 pr	888-958	3.0-4.0	-49.932±0.500	-4230.442
AH	Goldsmith and Newton, 1977	Solid-medium Pressure Apparatus	5 pr	1123-1173	1.0-15.0	3.598±0.015	-4230.696
AJ	Boettcher, 1970	Gas-medium Pressure Apparatus	2 pr	853-933	4.0-5.3	-212.732±2.710	-4230.933
AJ	Strens, 1968	Gas-medium Pressure Apparatus	1 pr	770-823	2.0	-219.358±5.645	-4232.259
AJ	Newton, 1966b	Gas-medium Pressure Apparatus	8 pr	758-1042	2.0-8.0	-209.387±4.619	-4230.267
AM	Storre and Nitsch, 1974	Gas- and Solid-medium Pressure Apparatus	2 pr	788-833	4.0-5.0	-88.085±1.706	-4230.358
AN	Chatterjee, 1971	Gas-medium Pressure Apparatus	3 pr	763-973	2.0-6.0	-94.229±1.257	-4230.284
AN	Chatterjee, 1974	Gas-medium Pressure Apparatus	5 pr	743-913	1.0-7.0	-94.010±0.933	-4230.065
AN	Storre and Nitsch, 1974	Gas- and Solid-medium Pressure Apparatus	3 pr	783-933	3.0-7.0	-93.722±1.703	-4229.778
AO	Hays, 1966	Solid-medium Pressure Apparatus	4 pr	1473-1673	11.0-14.6	-6.335±1.964	-4230.879
AP	Boettcher, 1970	Gas-medium Pressure Apparatus	1 pr	1033-1053	1.0	-101.524±0.981	-4231.523
AP	Huckenholz, 1974	Unspecified	3 pr	1028-1263	1.0-6.0	-102.146±1.163	-4232.145
AQ	Liou, 1971	Gas-medium Pressure Apparatus	5 pr	708-828	1.0-5.0	-89.629±0.446	-4230.690
AY	Storre and Nitsch, 1974	Gas- and Solid-medium Pressure Apparatus	3 pr	803-933	5.0-9.0	-86.359±0.132	-4232.351
BD	Kay and Taylor, 1960	log K	1	1653	0.001	84.430±2.584	-4228.036
BI	Kay and Taylor, 1960	log K	1	1543	0.001	61.011±2.412	-4225.974
BO	Kracek and Neuvonen, 1952	Solution calorimetry, HF acid	1	347	0.001	43.470±0.581	-4229.648
BO	Anderson and Kleppa, 1969	Solution calorimetry, HF acid	1	970	0.001	3.793±1.296	-4229.204
	This Study						-4230.697

Table 220. Continued

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
Reactions:							
AE	$2\ Ca_3Al_2Si_3O_{12}$[grossular] + $6\ CaAl_2Si_2O_8$[anorthite] + Al_2O_3[corundum] + $3\ H_2O$[g] = $6\ Ca_2Al_3Si_3O_{12}(OH)$[zoisite]						
AF	$2\ Ca_3Al_2Si_3O_{12}$[grossular] = $CaAl_2Si_2O_8$[anorthite] + $Ca_2Al_2SiO_7$[gehlenite] + $3\ CaSiO_3$[wollastonite]						
AG	$2\ CaSiO_3$[wollastonite] + $CaAl_2Si_2O_8$[anorthite] = $Ca_3Al_2Si_3O_{12}$[grossular] + SiO_2[quartz, alpha]						
AG	$2\ CaSiO_3$[wollastonite] + $CaAl_2Si_2O_8$[anorthite] = $Ca_3Al_2Si_3O_{12}$[grossular] + SiO_2[quartz, beta]						
AH	$3\ CaAl_2Si_2O_8$[anorthite] + $CaCO_3$[calcite] = $Ca_4Al_6Si_6O_{24}CO_3$[meionite]						
AJ	$5\ CaAl_2Si_2O_8$[anorthite] + $Ca_3Al_2Si_3O_{12}$[grossular] + $2\ H_2O$[g] = $4\ Ca_2Al_3Si_3O_{12}(OH)$[zoisite] + SiO_2[quartz, alpha]						
AM	Al_2SiO_5[andalusite] + $CaAl_2Si_2O_8$[anorthite] + H_2O[g] = $CaAl_4Si_2O_{10}(OH)_2$[margarite] + SiO_2[quartz, alpha]						
AN	$CaAl_2Si_2O_8$[anorthite] + Al_2O_3[corundum] + H_2O[g] = $CaAl_4Si_2O_{10}(OH)_2$[margarite]						
AO	$CaAl_2Si_2O_8$[anorthite] + $Ca_2Al_2SiO_7$[gehlenite] + Al_2O_3[corundum] = $3\ CaAl_2SiO_6$[Ca-Al clinopyroxene]						
AP	$CaAl_2Si_2O_8$[anorthite] + $Ca_2Al_2SiO_7$[gehlenite] = $Ca_3Al_2Si_3O_{12}$[grossular] + Al_2O_3[corundum]						
AQ	$CaAl_2Si_2O_8$[anorthite] + $CaSiO_3$[wollastonite] + H_2O[g] = $Ca_2Al_2Si_3O_{10}(OH)_2$[prehnite]						
AY	$CaAl_2Si_2O_8$[anorthite] + Al_2SiO_5[kyanite] + H_2O[g] = $CaAl_4Si_2O_{10}(OH)_2$[margarite] + SiO_2[quartz, alpha]						
BD	$2\ CaAl_2Si_2O_8$[anorthite] = $Ca_2Al_2SiO_7$[gehlenite] + Al_2O_3[corundum] + $3\ SiO_2$[cristobalite, beta]						
BF	$CaSiO_3$[cyclowollastonite] + $CaAl_2Si_2O_8$[anorthite] = $Ca_2Al_2SiO_7$[gehlenite] + $2\ SiO_2$[cristobalite, beta]						
BO	$CaAl_2Si_2O_8$[anorthite] + $3\ H_2O$[l] = CaO[lime] + $2\ Al(OH)_3$[gibbsite] + $2\ SiO_2$[quartz, alpha]						
BU	Al_2SiO_5[kyanite] + $CaSiO_3$[wollastonite] = $CaAl_2Si_2O_8$[anorthite]						

The relation between volumes and temperature as measured by high-temperature x-ray techniques differs considerably from the results using dilatometry. The weights were set such that the x-ray results were favored because the x-ray results are more precise and less subject to mechanical errors.

The heat capacities as measured by Robie and others (1978) and by Hemingway and others (1981) were used to determine the heat capacities, heat contents, and entropies below 1000 K. The experimental data of White (1919) and the smoothed results of Ferrier (1969) were used to obtain the same properties above 1000 K.

Several studies of the phase equilibria between anorthite and other minerals in the presence of quartz at pressures at and above 10 kb were not used in the evaluation. Goldsmith (1980) discusses the stoichiometry of anorthite and reports that stoichiometric anorthite will partially decompose to an alumina-deficient anorthite and corundum. Hays (1966) and Goldsmith (1980) studied the reaction

$$3\ CaAl_2Si_2O_8[\text{anorthite}] = Ca_3Al_2Si_3O_{12}[\text{grossular}] + 2\ Al_2SiO_5[\text{kyanite}] + SiO_2[\text{quartz}]$$

between 22 and 32.3 kb. The enthalpies of reaction at 298.15 K and 1.01 bars are -43.619 and -43.399 kJ, respectively. These lead to enthalpies of formation of -4223.529 and -4223.884 kJ/mol. These enthalpies of formation are very anomalous when compared to other data at lower pressure or data where corundum was a reactant or product.

1.5.5.14. $CaAl_4Si_2O_{10}(OH)_2$, margarite (formula weight = 398.186 g/mol)

Tables 221 and 222 contain the sources of data used in the final evaluation of the properties of margarite. In evaluating the heat capacity of margarite, the smoothed, composition-corrected data of Perkins and others (1980) were used.

The data used to evaluate the thermochemical properties are in good agreement. Only the reversal at 9 kb in the study by Storre and Nitsch (1974) is found to be in serious disagreement with the fitted properties.

1.5.5.15. $CaCO_3$ (formula weight = 100.089 g/mol)

The phase calcite is the stable phase at 1.01 bars. Therefore, the tables for calcite are used as the reference tables.

1.5.5.15.1. Calcite

Tables 223 and 224 contain the data used in the final evaluation. All other data, though cited in the reference list, were dropped before the final evaluation.

The volumetric properties were derived from the studies given in tables 223 and are in reasonable internal consistency. The heat capacities, heat contents, and the entropy of calcite are based primarily on the experimental data of Staveley and Linford (1969) and of Jacobs and others (1981). The compilation of Kelley (1960) was used to fix the properties above 800 K. Calcite has a number of polymorphs that have small differences in the crystal structure. Insuffi-

Table 221. Sources of thermophysical data for margarite, $CaAl_4Si_2O_{10}(OH)_2$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	0.02
Perkins and others, 1980	heat capacity	adiab. cal.	8	200-298	1.01	0.00±0.33
Perkins and others, 1980	heat capacity	d.s.c.	16	298-1000	1.01	-0.05±0.64
Perkins and others, 1980	entropy	adiab. cal.	1	298	1.01	-0.02

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 222. Sources of thermochemical data for margarite, $CaAl_4Si_2O_{10}(OH)_2$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
AM	Storre and Nitsch, 1974	Gas- and Solid-medium Pressure Apparatus	2 pr	788-833	4.0-5.0	-88.085±1.706	-6242.575
AN	Chatterjee, 1971	Gas-medium Pressure Apparatus	3 pr	763-973	2.0-6.0	-94.229±1.257	-6242.501
AN	Chatterjee, 1974	Gas-medium Pressure Apparatus	5 pr	743-913	1.0-7.0	-94.010±0.933	-6242.282
AN	Storre and Nitsch, 1974	Gas- and Solid-medium Pressure Apparatus	3 pr	783-933	3.0-7.0	-93.722±1.703	-6241.995
AY	Storre and Nitsch, 1974	Gas- and Solid-medium Pressure Apparatus	3 pr	803-933	5.0-9.0	-86.359±0.132	-6244.568
	This Study						-6242.914

Reactions:

AM Al_2SiO_5[andalusite] + $CaAl_2Si_2O_8$[anorthite] + H_2O[g] = $CaAl_4Si_2O_{10}(OH)_2$[margarite] + SiO_2[quartz, alpha]

AN $CaAl_2Si_2O_8$[anorthite] + Al_2O_3[corundum] + H_2O[g] = $CaAl_4Si_2O_{10}(OH)_2$[margarite]

AY $CaAl_2Si_2O_8$[anorthite] + Al_2SiO_5[kyanite] + H_2O[g] = $CaAl_4Si_2O_{10}(OH)_2$[margarite] + SiO_2[quartz, alpha]

Table 223. Sources of thermophysical data for calcite, $CaCO_3$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Adams and others, 1919	compressibility	dilatometry	17	298	1900-12000	-2.19±5.45
Rosenholtz and Smith, 1949	expansivity	dilatometry	7	373-973	1.01	6.87±41.38
Vaidya and others, 1973	volume	dilatometry	6	298	1.01-15000	0.13±0.37
Mirwald, 1979	volume	X-ray	3	903-1148	1.01	1.74±0.43
Kelley, 1960	heat content	compilation	9	400-1200	1.01	-0.38±1.81
Jacobs and others, 1981	heat capacity	d.s.c.	122	345-780	1.01	0.03±0.46
Staveley and Linford, 1969	heat capacity	adiab. cal.	10	222-303	1.01	0.22±0.25
Staveley and Linford, 1969	entropy	adiab. cal.	1	298	1.01	-0.08

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 224. Sources of thermochemical data for calcite, $CaCO_3$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H_r°(298.15 K) Third Law, kJ	H_f°(298.15 K) kJ/mol
AH	Goldsmith and Newton, 1977	Solid-medium Pressure Apparatus	5 pr	1123-1173	1.0-15.0	3.598±0.015	-1209.056
AI	Boettcher and Wyllie, 1968	Solid-medium Pressure Apparatus	2 pr	673	8.2-8.6	-0.822±0.049	-1209.277
AI	Boettcher and Wyllie, 1968	Solid-medium Pressure Apparatus	5 pr	753-1073	9.0-20.1	-0.730±0.336	-1209.185
AI	Goldsmith and Newton, 1969	Gas- and Solid-medium Pressure Apparatus	3 pr	673-723	8.5-10.5	-0.687±0.111	-1209.141
AI	Goldsmith and Newton, 1969	Gas- and Solid-medium Pressure Apparatus	10 pr	773-973	10.0-11.5	-0.755±0.134	-1209.209
AI	Johannes and Puhan, 1971	Gas-medium Pressure Apparatus	10	403-643	4.0-8.5	-0.591±0.116	-1209.046
AI	Johannes and Puhan, 1971	Gas-medium Pressure Apparatus	34	633-873	8.4-15.5	-0.547±0.138	-1209.002
AU	Baker, 1962	Vapor Pressure	21	1171-1458	0.001-0.025	180.525±0.552	-1209.871
AU	Smyth and Adams, 1923	Vapor Pressure, D.T.A.	12	1115-1355	0.00045-0.0089	180.010±1.076	-1209.385
	This Study						-1209.058

Reactions:

AH $3\ CaAl_2Si_2O_8$[anorthite] + $CaCO_3$[calcite] = $Ca_4Al_6Si_6O_{24}CO_3$[meionite]

AI $CaCO_3$[calcite] = $CaCO_3$[aragonite]

AU $CaCO_3$[calcite] = CaO[lime] + CO_2[g]

cient data exists to evaluate the properties of the individual polymorphs. Therefore, the tabulated data in tables 54, 55, and 160 represent the average properties of all the polymorphs of the calcite-related structural type.

The enthalpy of formation from the oxides is based on the decomposition data of Smyth and Adams (1923) and Baker (1962). These sets are in good agreement. However, the experiments of Harker and Tuttle (1955) lead to an enthalpy of reaction at 298.15 K of 170.564 ± 4.531 kJ/mol, a departure from the evaluated result of -9.773 kJ/mol.

1.5.5.15.2. Aragonite

Tables 225 and 226 contain the data used in the final evaluation. All other data, though cited in the reference list, were dropped before the final evaluation.

The calcite-aragonite reaction has been studied extensively. The data used (table 226) cover a large range in both temperature and pressure and are internally consistent.

1.5.5.16. CaO, lime (formula weight = 56.079 g/mol)

Except for the volumetric data, the properties of lime were taken from the JANAF Thermochemical Tables (Stull and Prophet, 1971). Table 227 gives the sources of data for the volumetric properties that were used in this study.

1.5.5.17. $CaSiO_3$ (formula weight = 116.164 g/mol)

The two polymorphs included in this study are wollastonite and cyclowollastonite (or "pseudowollastonite").

Table 225. Sources of thermophysical data for aragonite, $CaCO_3$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Kozu and Kani, 1934	volume	dilatometry	13	323-723	1.01	-1934±3.36
Vaidya and others, 1973	volume	dilatometry	6	298	1.01-15000	-0.64±0.41
Kelley, 1960	heat content	compilation	6	350-600	1.01	-0.13±0.10
Staveley and Lingford, 1969	heat capacity	adiab. cal.	9	206-291	1.01	0.06±0.37
Staveley and Lingford, 1969	entropy	adiab. cal.	1	298	1.01	-0.05±0.00

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 226. Sources of thermochemical data for aragonite, $CaCO_3$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_f(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
A1	Boettcher and Wyllie, 1968	Solid-medium Pressure Apparatus	2 pr	673	8.2-8.6	-0.822±0.049	-1209.880
A1	Boettcher and Wyllie, 1968	Solid-medium Pressure Apparatus	5 pr	753-1073	9.0-20.1	-0.730±0.336	-1209.788
A1	Goldsmith and Newton, 1969	Gas- and Solid-medium Pressure Apparatus	3 pr	673-723	8.5-10.5	-0.687±0.111	-1209.744
A1	Goldsmith and Newton, 1969	Gas- and Solid-medium Pressure Apparatus	10 pr	773-973	10.0-11.5	-0.755±0.134	-1209.812
A1	Johannes and Puhan, 1971	Gas-medium Pressure Apparatus	10	403-643	4.0-8.5	-0.591±0.116	-1209.649
A1	Johannes and Puhan, 1971	Gas-medium Pressure Apparatus	34	633-873	8.4-15.5	-0.547±0.138	-1209.605
	This Study						-1209.660

Reactions:

A1 $CaCO_3$[calcite] = $CaCO_3$[aragonite]

Table 227. Sources of volumetric data for lime, CaO.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Weir, 1956	V-V(2000 kb)	X-ray	9	294	2000-10000	2.35±6.23
Grain and Campbell, 1962	volume	X-ray	5	528-1398	1.01	0.00±0.03
Robie and others, 1967	volume	compilation	1	298	1.01	0.017
Swanson and Tatge, 1953	volume	X-ray	1	300	1.01	-0.011

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

1.5.5.17.1. Wollastonite

Tables 228 and 229 contain the sources of data used in the final evaluation of the properties of wollastonite. All other data, though given in the reference list, were dropped before the final evaluation.

The heat capacity data that were given the highest weight in the evaluation were the data from adiabatic calorimetry and differential scanning calorimetry (d.s.c.) by Krupka and others (1980) and the data above 1000 K from the drop calorimetry of Southard (1941).

The thermochemical data used are in good internal agreement. The most divergent data seem to be from the borate-salt solution calorimetry. However, even here the departure in enthalpy of formation from the elements is only 2 kJ/mol. The thermochemical properties of wollastonite were also controlled by the evaluation of the data for cyclowollastonite and the forcing of an inversion temperature of 1398.15 K (Osborn and Schairer, 1941) where the Gibbs energy difference between the two polymorphs is forced to be zero.

1.5.5.17.2. Cyclowollastonite (= "pseudowollastonite")

Tables 230 and 231 contain the data in the final evaluation. Other data, though cited in the reference list, were dropped prior to the final evaluation.

The reported inversion temperature at 1.01 bars is 1398.15 ± 10 K (Osborn and Schairer, 1941). The thermochemical properties were determined from the tabulated data relating to cyclowollastonite and wollastonite using the inversion temperature as a fixed point where the Gibbs energies of the polymorphs are equal.

Table 228. Sources of thermophysical data for wollastonite, $CaSiO_3$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Vaidya and others, 1973	volume diff.	dilatometry	9	298	3000-45000	0.00±0.05
Evans, Howard, 1977(unpub.)	volume	X-ray	7	303-873	1.01	-0.04±0.09
Cristescu and Simon, 1934	heat capacity	isotherm. cal.	2	200-210	1.01	1.93±0.06
Christescu, 1931	heat capacity	isotherm. cal.	7	199-303	1.01	1.46±1.40
Krupka and others, 1980	heat capacity	adiab. cal.	39	200-386	1.01	-0.10±0.29
Gronow and Schweite, 1933	heat content	drop cal.	5	573-1373	1.01	-0.19±0.82
Southard, 1941	heat content	drop cal.	13	484-1418	1.01	0.07±0.40
Roth and Bertram, 1929	heat content	drop cal.	7	323-1157	1.01	-0.98±0.52
White, 1919	heat content	drop cal.	8	973-1573	1.01	-0.45±0.46
White, 1919	heat content	drop cal.	10	373-973	1.01	1.31±1.01
Wagner, 1932	heat content	drop cal.	11	566-1369	1.01	-0.18±0.82
Krupka and others, 1980	heat capacity	d.s.c.	99	349-999	1.01	0.16±0.66
Hemingway and Robie, 1977	entropy	compilation	1	298	1.01	0.64

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 229. Sources of thermochemical data for wollastonite, $CaSiO_3$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
AF	Hays, 1966	Solid-medium Pressure Apparatus	2 pr	1473-1523	7.5-11.0	-157.994±6.068	-1634.000
AF	Huckenholz, 1974	Unspecified	6 pr	1125-1423	0.2-7.5	-158.840±1.799	-1634.282
AF	Shmulovich, 1974	Gas-medium Pressure Apparatus	1 pr	1133-1153	0.506	-159.474±1.420	-1634.809
AG	Boettcher, 1970	Gas-medium Pressure Apparatus	2 pr	893-1053	3.0-5.9	-50.204±1.453	-1634.643
AG	Newton, 1966b	Gas-medium Pressure Apparatus	2 pr	803-923	1.1-2.0	-51.867±3.013	-1635.778
AG	Newton, 1966b	Gas-medium Pressure Apparatus	2 pr	973-1023	4.7-5.7	-48.971±1.851	-1634.043
AG	Huckenholz, 1974	Unspecified	1 pr	848-858	2.0	-49.455±0.327	-1634.572
AG	Huckenholz, 1974	Unspecified	2 pr	888-958	3.0-4.0	-49.932±0.500	-1634.523
AQ	Liou, 1971	Gas-medium Pressure Apparatus	5 pr	708-828	1.0-5.0	-89.629±0.446	-1634.644
BH	Benz and Wagner, 1961	E.M.F.	12	898-1148	0.001	-43.707±0.175	-1634.208
BN	Essene, 1974	Solid-medium Pressure Apparatus	3 pr	1723-1833	13.0-20.0	6.183±0.044	-1634.610
BN	Huang and Wyllie, 1975	Solid-medium Pressure Apparatus	1 pr	1823	21.0-22.0	6.150±0.043	-1634.642
BN	Charlu and others, 1978	Solution calorimtery, borate salt	1	970	0.001	8.215±0.779	-1632.577
BN	Kiseleva and others, 1979	Solution calorimetry, borate salt	1	1070	0.001	8.245	-1632.547
BN	Kracek and others, 1953	Solution calorimetry, HF acid	1	298	0.001	6.525	-1633.774
BN	Nacken, 1930	Solution calorimetry, HF acid	5	314	0.001	8.128±1.098	-1632.664
BP	Charlu and others, 1978	Solution calorimetry, borate salt	1	970	0.001	67.438±1.972	-1636.440
BU	Anderson and Kleppa, 1969	Solution calorimetry, borate salt	1	970	0.001	3.793±1.296	-1633.158
BX	Barany, 1966	Solution calorimetry, HF acid	5	347	0.001	89.764±0.237	-1633.774
	This Study						-1634.651

Table 229. Continued

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_f(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
Reactions:							
AF	$2\ Ca_3Al_2Si_3O_{12}$[grossular] = $CaAl_2Si_2O_8$[anorthite] + $Ca_2Al_2SiO_7$[gehlenite] + 3 $CaSiO_3$[wollastonite]						
AG	2 $CaSiO_3$[wollastonite] + $CaAl_2Si_2O_8$[anorthite] = $Ca_3Al_2Si_3O_{12}$[grossular] + SiO_2[quartz, alpha]						
AG	2 $CaSiO_3$[wollastonite] + $CaAl_2Si_2O_8$[anorthite] = $Ca_3Al_2Si_3O_{12}$[grossular] + SiO_2[quartz, beta]						
AQ	$CaAl_2Si_2O_8$[anorthite] + $CaSiO_3$[wollastonite] + H_2O[g] = $Ca_2Al_2Si_3O_{10}(OH)_2$[prehnite]						
BH	CaO[lime] + SiO_2[quartz, beta] = $CaSiO_3$[wollastonite]						
BN	$CaSiO_3$[wollastonite] = $CaSiO_3$[cyclowollastonite]						
BP	$Ca_3Al_2Si_3O_{12}$[grossular] = $CaAl_2SiO_6$[Ca-Al clinopyroxene] + 2 $CaSiO_3$[wollastonite]						
BU	Al_2SiO_5[kyanite] + $CaSiO_3$[wollastonite] = $CaAl_2Si_2O_8$[anorthite]						
BX	$CaSiO_3$[wollastonite] = CaO[lime] + SiO_2[quartz, alpha]						

Table 230. Sources of thermophysical data for cyclowollastonite, $CaSiO_3$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Evans, Howard, 1977(unpub.)	volume	X-ray	7	303-873	1.01	-0.08±0.21
Vaidya and others, 1973	volume	dilatometry	9	298	5000-45000	0.05±0.10
Robie and others, 1979	volume	compilation	1	298	1.01	-0.19
Wagner, 1932	heat content	drop cal.	12	576-1558	1.01	1.93±0.67
Wagner, 1932	heat capacity	isotherm. cal.	7	201-295	1.01	-0.68±1.77
White, 1919	heat content	drop cal.	28	373-1673	1.01	1.54±1.44
Parks and Kelley, 1926	heat capacity	isotherm. cal.	6	194-298	1.01	-0.38±0.70
Hemingway and Robie, 1977	entropy	compilation	1	298	1.01	0.199

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 231. Sources of thermochemical data for cyclowollastonite (= "pseudowollastonite"), $CaSiO_3$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H_r°(298.15 K) Third Law, kJ	H_f°(298.15 K) kJ/mol
BE	Kay and Taylor, 1960	log K	1	1773	0.001	-87.895±2.771	-1628.937
BF	Kay and Taylor, 1960	log K	1	1543	0.001	61.011±2.412	-1623.787
BG	Benz and Wagner, 1961	E.M.F.	10	943-1003	0.001	-41.476±0.186	-1628.505
BN	Essene, 1974	Solid-medium Pressure Apparatus	3 pr	1723-1833	13.0-20.0	6.183±0.044	-1628.469
BN	Huang and Wyllie, 1975	Solid-medium Pressure Apparatus	1 pr	1823	21.0-22.0	6.150±0.043	-1628.501
BN	Charlu and others, 1978	Solution calorimtery, borate salt	1	970	0.001	8.215±0.779	-1626.436
BN	Kiseleva and others, 1979	Solution calorimetry, borate salt	1	1070	0.001	8.245	-1626.406
BN	Kracek and others, 1953	Solution calorimetry, HF acid	1	298	0.001	6.525	-1628.894
BN	Nacken, 1930	Solution calorimetry, HF acid	5	314	0.001	8.128±1.098	-1626.523
	This Study						-1628.510

Reactions:

BE $CaO[lime] + SiO_2[cristobalite, beta] = CaSiO_3[cyclowollastonite]$

BF $CaSiO_3[cyclowollastonite] + CaAl_2Si_2O_8[anorthite] = Ca_2Al_2SiO_7[gehlenite] + 2\ SiO_2[cristobalite, beta]$

BG $2\ CaSiO_3[cyclowollastonite] + CaO[lime] = Ca_3Si_2O_7[rankinite]$

BN $CaSiO_3[wollastonite] = CaSiO_3[cyclowollastonite]$

1.5.5.18. $Ca_2Al_2SiO_6(OH)_2$, bicchulite (formula weight = 292.220 g/mol)

Tables 232 and 233 contain the data used in the final evaluation. Only the molar volume of bicchulite was available. The other properties were derived from the fictive-component method of estimation as cited in section 1.3.2 or by the slope of the univariant reaction in pressure-temperature space. The large 2-sigma confidence limits given on the tables reflect this lack of available data.

1.5.5.19. $Ca_2Al_2SiO_6$, gehlenite (formula weight = 274.204 g/mol)

Tables 234 and 235 contain the data used in the final evaluation of the properties of gehlenite. All other data, though cited in the reference list, were dropped before the final evaluation.

The enthalpy of solution of gehlenite in HF acid solutions as measured by Barany (1963) was probably obtained from a sample that, at the time of measurement, was not gehlenite even though it had been so identified before grinding and sizing by siltation in water. Gehlenite, being one of the cement phases, may have reacted with the water during the siltation and not converted back to gehlenite during drying at 973 K. In any event, the results Barany achieved were what would be expected if one were working with a metastable or reacted material. They are discordant with the entropy and phase equilibria for gehlenite.

Table 232. Sources of thermophysical data for bicchulite, $Ca_2Al_2SiO_6(OH)_2$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Gupta and Chatterjee, 1978	volume	X-ray	1	298	1.01	-0.05

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 233. Sources of thermochemical data for bicchulite, $Ca_2Al_2SiO_6(OH)_2$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
AS	Gupta and Chatterjee, 1978	Gas-medium Pressure Apparatus	7 pr	890-1033	0.5-7.05	112.694±0.646	-4336.660
AS	Huckenholz, 1977	Unspecified	8 pr	884-1023	0.5-7.0	111.563±0.725	-4337.790
	This Study						-4337.238

Reactions:

AS $Ca_2Al_2SiO_6(OH)_2$[bicchulite] = $Ca_2Al_2SiO_7$[gehlenite] + H_2O[g]

Table 234. Sources of thermophysical data for gehlenite, $Ca_2Al_2SiO_7$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	-0.01
Weller and Kelley, 1963	heat capacity	isotherm. cal.	10	206-296	1.01	-0.03±0.07
Pankratz and Kelley, 1964a	heat content	drop cal.	15	402-1801	1.01	0.01±0.17
Hemingway and Robie, 1977	entropy	compilation	1	978	1.01	-0.097

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 235. Sources of thermochemical data for gehlenite, $Ca_2Al_2SiO_7$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_0(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
AF	Hays, 1966	Solid-medium Pressure Apparatus	2 pr	1473-1523	7.5-11.0	-157.994±6.068	-3981.332
AF	Huckenholz, 1974	Unspecified	6 pr	1125-1423	0.2-7.5	-158.840±1.799	-3982.178
AF	Shmulovich, 1974	Gas-medium Pressure Apparatus	1 pr	1133-1153	0.506	-159.474±1.420	-3983.760
AO	Hays, 1966	Solid-medium Pressure Apparatus	4 pr	1473-1673	11.0-14.6	-6.335±1.964	-3983.468
AP	Boettcher, 1970	Gas-medium Pressure Apparatus	1 pr	1033-1053	1.0	-101.624±0.981	-3984.112
AP	Huckenholz, 1974	Unspecified	3 pr	1028-1263	1.0-6.0	-102.146±1.163	-3984.723
AS	Gupta and Chatterjee, 1978	Gas-medium Pressure Apparatus	7 pr	890-1033	0.5-7.05	112.694±0.646	-3982.708
AS	Huckenholz, 1977	Unspecified	8 pr	884-1023	0.5-7.0	111.563±0.725	-3983.838
BD	Kay and Taylor, 1960	log K	1	1653	0.001	84.430±2.584	-3980.625
BF	Kay and Taylor, 1960	log K	1	1543	0.001	61.011±2.412	-3978.563
	This Study						-3983.286

Reactions:

AF $2\ Ca_3Al_2Si_3O_{12}$[grossular] = $CaAl_2Si_2O_8$[anorthite] + $Ca_2Al_2SiO_7$[gehlenite] + $3\ CaSiO_3$[wollastonite]

AO $CaAl_2Si_2O_8$[anorthite] + $Ca_2Al_2SiO_7$[gehlenite] + Al_2O_3[corundum] = $3\ CaAl_2SiO_6$[Ca-Al clinopyroxene]

AP $CaAl_2Si_2O_8$[anorthite] + $Ca_2Al_2SiO_7$[gehlenite] = $Ca_3Al_2Si_3O_{12}$[grossular] + Al_2O_3[corundum]

AS $Ca_2Al_2SiO_6(OH)_2$[bicchulite] = $Ca_2Al_2SiO_7$[gehlenite] + H_2O[g]

BD $2\ CaAl_2Si_2O_8$[anorthite] = $Ca_2Al_2SiO_7$[gehlenite] + Al_2O_3[corundum] + $3\ SiO_2$[cristobalite, beta]

BF $CaSiO_3$[cyclowollastonite] + $CaAl_2Si_2O_8$[anorthite] = $Ca_2Al_2SiO_7$[gehlenite] + $2\ SiO_2$[cristobalite, beta]

1.5.5.20. $Ca_2Al_2Si_3O_{10}(OH)_2$, prehnite (formula weight = 412.388 g/mol)

Tables 236 and 237 contain the sources of data used to evaluate the properties of prehnite. The smoothed, composition-corrected heat capacities of Perkins and others (1980) were used in the evaluation.

Only the study by Liou (1971) on the equilibria among anorthite, wollastonite, prehnite, and H_2O[gas] had a slope that was consistent with the entropy and molar volume. All other studies were therefore discarded.

1.5.5.21. $Ca_2Al_3Si_3O_{12}(OH)$, zoisite (formula weight = 454.361 g/mol)

Tables 238 and 239 contain the sources of data used in the final evaluation. All other data, though cited in the reference list, were deleted prior to the final evaluation. The smoothed, composition-corrected heat capacities measured by Perkins and others (1980) were used for the final evaluation.

The thermochemical data are in good agreement. The apparently discordant study by Strens (1968) on table 239 is due to the wide temperature bracket for the phase equilibrium reversal of about 53 kelvins. The refined properties lie within the reversal bracket at 2 kb and are consistent with it.

1.5.5.22. Ca_2SiO_4 (formula weight = 172.243 g/mol)

Tables 240 through 245 contain the data used in the final evaluation for the Ca_2SiO_4 polymorphs Ca olivine, bredigite, larnite, and

Table 236. Sources of thermophysical data for prehnite, $Ca_2Al_2Si_3O_{10}(OH)_2$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	-0.08
Perkins and others, 1980	heat capacity	adiab. cal.	8	200-298	1.01	0.00±0.05
Perkins and others, 1980	heat capacity	d.s.c.	12	298-800	1.01	-0.08±0.23
Perkins and others, 1980	entropy	adiab. cal.	1	298	1.01	0.001

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 237. Sources of thermochemical data for prehnite, $Ca_2Al_2Si_3O_{10}(OH)_2$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Pressure (kb)	H_r°(298.15 K) Third Law, kJ	H_f°(298.15 K) kJ/mol
AQ	Liou, 1971	Gas-medium Pressure Apparatus	5 pr	708-828	1.0-5.0	-89.629±0.446	-6196.813
	This Study						-6196.820

Reactions:

AQ $CaAl_2Si_2O_8$[anorthite] + $CaSiO_3$[wollastonite] + H_2O[g] = $Ca_2Al_2Si_3O_{10}(OH)_2$[prehnite]

Table 238. Sources of thermophysical data for zoisite, $Ca_2Al_3Si_3O_{12}(OH)$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	-0.15
Perkins and others, 1980	heat capacity	adiab. cal.	8	200-298	1.01	0.01±0.17
Perkins and others, 1980	heat capacity	d.s.c.	11	298-750	1.01	-0.72±0.71
Perkins and others, 1980	entropy	adiab. cal.	1	298	1.01	-0.015

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 239. Sources of thermochemical data for zoisite, $Ca_2Al_3Si_3O_{12}(OH)$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
AE	Newton, 1965	Gas- and Solid-medium Pressure Apparatus	6 pr	843-1113	2.0-6.8	-304.099±2.670	-6894.569
AE	Boettcher, 1970	Gas-medium Pressure Apparatus	1 pr	898-928	3.0	-305.304±3.803	-6894.769
AJ	Boettcher, 1970	Gas-medium Pressure Apparatus	2 pr	853-933	4.0-5.3	-212.732±2.710	-6894.540
AJ	Strens, 1968	Gas-medium Pressure Apparatus	1 pr	770-823	2.0	-219.358±5.645	-6896.197
AJ	Newton, 1966b	Gas-medium Pressure Apparatus	8 pr	758-1042	2.0-8.0	-209.387±4.619	-6893.704
	This Study						-6894.244

Reactions:

AE $2\ Ca_3Al_2Si_3O_{12}$[grossular] + $6\ CaAl_2Si_2O_8$[anorthite] + Al_2O_3[corundum] + $3\ H_2O$[g] = $6\ Ca_2Al_3Si_3O_{12}(OH)$[zoisite]

AJ $5\ CaAl_2Si_2O_8$[anorthite] + $Ca_3Al_2Si_3O_{12}$[grossular] + $2\ H_2O$[g] = $4\ Ca_2Al_3Si_3O_{12}(OH)$[zoisite] + SiO_2[quartz, alpha]

Table 240. Sources of thermophysical data for alpha-Ca_2SiO_4.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Douglas, 1952	volume	X-ray	1	298	1.01	0.0
Coughlin and O'Brien, 1957	heat content	drop cal.	5	1714-1816	1.01	0.0±0.10

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 241. Sources of thermophysical data for bredigite, Ca_2SiO_4.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	0.0
Coughlin and O'Brien, 1957	heat content	drop cal.	12	974-1690	1.01	0.02±0.14

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 242. Sources of thermochemical data for bredigite, Ca_2SiO_4.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
AR	Carlson, 1931	Phase Equilibria, Rapid Quench	1	1523	0.001	11.573±0.155	-2310.191
BI	Benz and Wagner, 1961	E.M.F.	10	971-1143	0.001	-5.080±0.376	-2310.149
	This Study						-2310.188

Reactions:

AR Ca_2SiO_4[bredigite] + CaO[lime] = Ca_3SiO_5[hatrurite]

BI CaO[lime] + $Ca_3Si_2O_7$[rankinite] = 2 Ca_2SiO_4[bredigite]

Table 243. Sources of thermophysical data for Ca-olivine, Ca_2SiO_4.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	0.0
King, 1957	heat capacity	isotherm. cal.	10	206-296	1.01	0.05±0.47
Coughlin and O'Brien, 1957	heat content	drop cal.	18	405-1112	1.01	-0.25±0.91
King, 1957	entropy	isotherm. cal.	1	298	1.01	0.0

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 244. Sources of thermophysical data for larnite, Ca_2SiO_4.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Rigby and Green, 1942	volume diff.	dilatometry	11	473-1473	1.01	-0.03±2.00
Robie and others, 1979	volume	compilation	1	298	1.01	0.0
Todd, 1951	heat capacity	adiab. cal.	10	206-296	1.01	0.02±0.11
Coughlin and O'Brien, 1957	heat content	drop cal.	10	406-965	1.01	-0.02±0.16
Hemingway and Robie, 1977	entropy	compilation	1	298	1.01	0.37

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 245. Sources of thermochemical data for larnite, Ca_2SiO_4.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
BJ	Benz and Wagner, 1961	E.M.F.	3	943-963	0.001	-2.298±0.087	-2307.152
BV	King, 1951	Solution calorimetry, HF acid	1	347	0.001	126.660±1.093	-2306.930
BW	Brunauer and others, 1956	Solution calorimetry, HF-HNO3 acid	1	296	0.001	-8.676±0.926	-2307.286
	This Study						-2307.224

Reactions:

BJ $CaO[lime] + Ca_3Si_2O_7[rankinite] = 2\ Ca_2SiO_4[larnite]$

BV $Ca_2SiO_4[larnite] = SiO_2[quartz,\ alpha] + 2\ CaO[lime]$

BW $Ca_3SiO_5[hatrurite] = Ca_2SiO_4[larnite] + CaO[lime]$

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a high-temperature phase often referred to as alpha-Ca_2SiO_4. The inversion temperatures are as follows:

Ca olivine = bredigite	1120 K
bredigite = alpha-Ca_2SiO_4	1710 K
larnite = bredigite	970 K

The stability relations are best shown by the Gibbs energy - temperature plot (figure 8) where it is readily recognized that larnite is metastable at 1.01 bars at all temperatures between 200 and 1800 K.

1.5.5.22.1. Alpha-Ca_2SiO_4

For alpha-Ca_2SiO_4, the thermochemical properties were derived from the thermophysical properties, the inversion temperatures, and the phase equilibria with the other polymorphs.

1.5.5.22.2. Bredigite

For bredigite, the thermochemical properties were derived from the thermophysical properties, the inversion temperatures, and the phase equilibria with the other polymorphs, and with rankinite and hatrurite.

1.5.5.22.3. Ca olivine

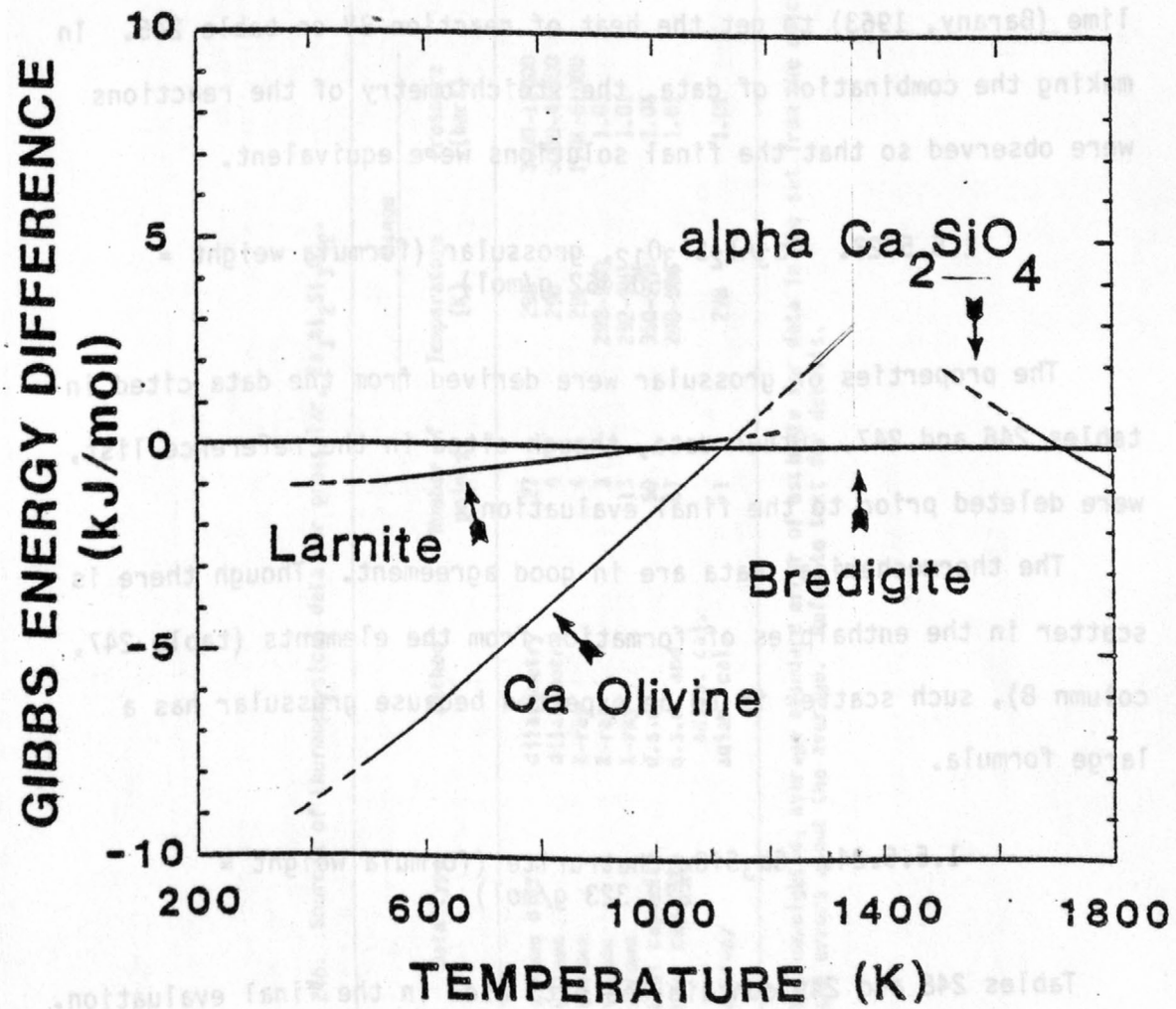
For Ca olivine, the thermochemical properties were derived from the thermophysical properties, the inversion temperatures, and the phase equilibria for the other polymorphs.

1.5.5.22.4. Larnite

For larnite, the thermochemical properties were derived from the thermophysical properties, the inversion temperatures, the phase

Figure 8. Gibbs energy difference of phases indicated relative to bredigite at 1.01 bars. The phase with the most negative Gibbs energy difference is the stable phase at temperature and 1.01 bars. Ca olivine is the stable phase up to 1120 K. Bredigite is stable between 1120 and 1710 K. Above 1710, alpha-Ca_2SiO_4 is stable. Larnite is more stable than bredigite below 970 K but less stable than Ca olivine.

Figure 8, Robinson and others



equilibria with other calcium silicates, and solution calorimetry. Concerning the latter data, King (1951) measured the heat of solution of larnite in HF acid. These data were combined with the heats of solution of quartz (Bennington and others, 1978) and of 2 moles of lime (Barany, 1963) to get the heat of reaction BV on table 245. In making the combination of data, the stoichiometry of the reactions were observed so that the final solutions were equivalent.

1.5.5.23. $Ca_3Al_2Si_3O_{12}$, grossular (formula weight = 450.452 g/mol)

The properties of grossular were derived from the data cited in tables 246 and 247. Other data, though cited in the reference list, were deleted prior to the final evaluation.

The thermochemical data are in good agreement. Though there is scatter in the enthalpies of formation from the elements (table 247, column 8), such scatter is to be expected because grossular has a large formula.

1.5.5.24. Ca_3SiO_5, hatrurite (formula weight = 228.323 g/mol)

Tables 248 and 249 contain the data used in the final evaluation. The heat-capacity and heat-content data are too widely spaced to evaluate the properties of the individual polymorphs. The tabulated data in tables 86, 87, and 174, therefore, represent the average properties of all the polymorphs.

The heat of solution of hatrurite relative to a mechanical mixture of larnite and lime is in excellent agreement with the heat content

Table 246. Sources of thermophysical data for grossular, $Ca_3Al_2Si_3O_{12}$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Adams and Gibson, 1929	volume diff.	dilatometry	27	298	3000-12000	4.64±7.23
Vaidya and others, 1973	volume	dilatometry	9	298	5000-45000	-0.01±0.05
Hazen and Finger, 1978	volume	X-ray	4	296	1.01-61000	-0.04±0.03
Meagher, 1975	volume	X-ray	3	298-940	1.01	0.04±0.09
Skinner, 1956	volume	X-ray	13	292-981	1.01	0.01±0.05
Krupka and others, 1979	heat capacity	d.s.c.	50	350-978	1.01	0.71±1.23
Westrum and others, 1979	heat capacity	d.s.c. and adiab. cal.	57	200-596	1.01	-0.01±0.20
Westrum and others, 1979	entropy	adiab. cal.	1	298	1.01	0.554

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 247. Sources of thermochemical data for grossular, $Ca_3Al_2Si_3O_{12}$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_f(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
AE	Newton, 1965	Gas- and Solid-medium Pressure Apparatus	6 pr	843-1113	2.0-6.8	-304.099±2.670	-6639.916
AE	Boettcher, 1970	Gas-medium Pressure Apparatus	1 pr	898-928	3.0	-305.304±3.803	-6640.519
AF	Hays, 1966	Solid-medium Pressure Apparatus	2 pr	1473-1523	7.5-11.0	-157.994±6.068	-6637.966
AF	Huckenholz, 1974	Unspecified	6 pr	1125-1423	0.2-7.5	-158.840±1.799	-6638.389
AF	Shmulovich, 1974	Gas-medium Pressure Apparatus	1 pr	1133-1153	0.506	-159.474±1.420	-6639.180
AG	Boettcher, 1970	Gas-medium Pressure Apparatus	2 pr	893-1053	3.0-5.9	-50.204±1.453	-6638.959
AG	Newton, 1966b	Gas-medium Pressure Apparatus	2 pr	803-923	1.1-2.0	-51.867±3.013	-6641.197
AG	Newton, 1966b	Gas-medium Pressure Apparatus	2 pr	973-1023	4.7-5.7	-48.971±1.851	-6637.727
AG	Huckenholz, 1974	Unspecified	1 pr	848-858	2.0	-49.455±0.327	-6638.786
AG	Huckenholz, 1974	Unspecified	2 pr	888-958	3.0-4.0	-49.932±0.500	-6638.688
AI	Gasparik, 1981	Solid-medium Pressure Apparatus	3 pr	1463-1673	10.75-23.5	-94.622±2.588	-6639.020
AJ	Boettcher, 1970	Gas-medium Pressure Apparatus	2 pr	853-933	4.0-5.3	-212.732±2.710	-6640.127
AJ	Strens, 1968	Gas-medium Pressure Apparatus	1 pr	770-823	2.0	-219.358±5.645	-6646.753
AJ	Newton, 1966b	Gas-medium Pressure Apparatus	8 pr	758-1042	2.0-8.0	-209.387±4.619	-6636.783
AP	Boettcher, 1970	Gas-medium Pressure Apparatus	1 pr	1033-1053	1.0	-101.524±0.981	-6639.769
AP	Huckenholz, 1974	Unspecified	3 pr	1028-1263	1.0-6.0	-102.146±1.163	-6640.391
BP	Charlu and others, 1978	Solution calorimetry, borate salt	1	970	0.001	67.438±1.972	-6642.531
	This Study						-6638.943

Table 247. Continued

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
Reactions:							
AL	$2\ Ca_3Al_2Si_3O_{12}$[grossular] + $6\ CaAl_2Si_2O_8$[anorthite] + Al_2O_3[corundum] + $3\ H_2O$[g] = $6\ Ca_2Al_3Si_3O_{12}(OH)$[zoisite]						
AF	$2\ Ca_3Al_2Si_3O_{12}$[grossular] = $CaAl_2Si_2O_8$[anorthite] + $Ca_2Al_2SiO_7$[gehlenite] + $3\ CaSiO_3$[wollastonite]						
AG	$2\ CaSiO_3$[wollastonite] + $CaAl_2Si_2O_8$[anorthite] = $Ca_3Al_2Si_3O_{12}$[grossular] + SiO_2[quartz, alpha]						
AG	$2\ CaSiO_3$[wollastonite] + $CaAl_2Si_2O_8$[anorthite] = $Ca_3Al_2Si_3O_{12}$[grossular] + SiO_2[quartz, beta]						
AI	$3\ CaAl_2SiO_6$[Ca-Al clinopyroxene] = $Ca_3Al_2Si_3O_{12}$[grossular] + $2\ Al_2O_3$[corundum]						
AJ	$5\ CaAl_2Si_2O_8$[anorthite] + $Ca_3Al_2Si_3O_{12}$[grossular] + $2\ H_2O$[g] = $4\ Ca_2Al_3Si_3O_{12}(OH)$[zoisite] + SiO_2[quartz, alpha]						
AP	$CaAl_2Si_2O_8$[anorthite] + $Ca_2Al_2SiO_7$[gehlenite] = $Ca_3Al_2Si_3O_{12}$[grossular] + Al_2O_3[corundum]						
BP	$Ca_3Al_2Si_3O_{12}$[grossular] = $CaAl_2SiO_6$[Ca-Al clinopyroxene] + $2\ CaSiO_3$[wollastonite]						

Table 248. Sources of thermophysical data for hatrurite, Ca_3SiO_5.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Rigby and Green, 1942	expansivity	dilatometry	11	473-1473	1.01	0.00±3.13
Yamaguchi and Miyabe, 1960	volume	X-ray	1	298	1.01	0.0
Todd, 1951	heat capacity	isotherm. cal.	9	206-296	1.01	0.00±0.11
Gronow and Schweite, 1933	heat content	drop cal.	7	573-1173	1.01	0.44±0.54
Todd, 1951	entropy	isotherm. cal.	1	298	1.01	0.001

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 249. Sources of thermochemical data for hatrurite, Ca_3SiO_5.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H_r°(298.15 K) Third Law, kJ	H_f°(298.15 K) kJ/mol
AR	Carlson, 1931	Phase Equilibria, Rapid Quench	1	1523	0.001	11.573±0.155	-2933.707
BW	Brunauer and others, 1956	Solution calorimetry, HF-HNO3 acid	1	296	0.001	-8.676±0.926	-2933.766
	This Study						-2933.704

Reactions:

AR Ca_2SiO_4[bredigite] + CaO[lime] = Ca_3SiO_5[hatrurite]

BW Ca_3SiO_5[hatrurite] = Ca_2SiO_4[larnite] + CaO[lime]

data for the three phases and the breakdown temperature of 1523 ± 25 K observed by Carlson (1931). The departure is 0.35 kelvins for a calculated breakdown temperature of 1523.5 K.

1.5.5.25. $Ca_3Si_2O_7$, rankinite (formula weight = 288.407 g/mol)

Tables 250 and 251 contain the data used in the final evaluation. It should be pointed out that the data used for adjusting the thermochemical properties of rankinite are limited to e.m.f. studies. However, other data provided by this source for larnite, bredigite, and wollastonite are in good agreement with data from other sources. It is assumed that these data are also of high quality.

1.5.5.26. $Ca_4Al_6Si_6O_{24}(CO_3)$, meionite (formula weight = 931.717 g/mol)

Tables 252 and 253 contain the sources of data for the evaluation of properties of meionite. The errors on the property tables reflect the lack of detailed experimental data that are necessary to provide a more accurate evaluation. Especially needed are data on the entropy and heat capacity.

1.5.5.27. Fe, iron (formula weight = 55.847 g/mol)

The thermodynamic properties of iron were taken from the JANAF Thermochemical Tables[a]. The molar volume was not needed in this study and therefore not evaluated.

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[a]JANAF Thermochemical Tables, looseleaf pages for 1978 issued by Dow Chemical Company, 1707 Building, Midland, Michigan.

Table 250. Sources of thermophysical data for rankinite, $Ca_3Si_2O_7$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Rigby and Green, 1942	volume diff.	dilatometry	11	473-1473	1.01	-0.17±2.68
Saburi and others, 1976	volume	X-ray	1	298	1.01	0.0
King, 1957	heat capacity	isotherm. cal.	10	206-296	1.01	0.00±0.15
King, 1957	entropy	isotherm. cal.	1	298	1.01	-0.441

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 251. Sources of thermochemical data for rankinite, $Ca_3Si_2O_7$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
BG	Benz and Wagner, 1961	E.M.F.	10	943-1003	0.001	-41.476±0.186	-3975.040
BI	Benz and Wagner, 1961	E.M.F.	10	971-1143	0.001	-5.080±0.376	-3974.972
BJ	Benz and Wagner, 1961	E.M.F.	3	943-963	0.001	-2.298±0.087	-3974.906
	This Study						-3975.050

Reactions:

BG $2\ CaSiO_3$[cyclowollastonite] + CaO[lime] = $Ca_3Si_2O_7$[rankinite]

BI CaO[lime] + $Ca_3Si_2O_7$[rankinite] = $2\ Ca_2SiO_4$[bredigite]

BJ CaO[lime] + $Ca_3Si_2O_7$[rankinite] = $2\ Ca_2SiO_4$[larnite]

Table 252. Sources of thermophysical data for meionite, $Ca_4Al_6Si_6O_{24}CO_3$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Goldsmith and Newton, 1977	volume	X-ray	1	298	1.01	0.85

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 253. Sources of thermochemical data for melonite, $Ca_4Al_6Si_6O_{24}CO_3$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_f(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
All	Goldsmith and Newton, 1977	Solid-medium Pressure Apparatus	5 pr	1123-1173	1.0-15.0	3.598±0.015	-13897.547
	This Study						-13897.549

Reactions:

All 3 $CaAl_2Si_2O_8$[anorthite] + $CaCO_3$[calcite] = $Ca_4Al_6Si_6O_{24}CO_3$[melonite]

1.5.5.28. $Fe_{.947}O$, wustite (formula weight = 68.887 g/mol)

Tables 254 and 255 contain the sources of data used to evaluate the properties of wustite. All other data, though cited in the reference list, were deleted prior to the final evaluation.

The two composite sets of data for wustite-iron and wustite-magnetite equilibria were developed from the compositions of wustite that coexisted with iron or magnetite, respectively, as measured by Darken and Gurry (1945) and from the log $f(O_2)$-composition experiments of Vallet and Raccah (1965), Bransky and Hed (1968), and Lohberg and Stannek (1975).

The breakdown temperature determined by Rau (1972) by H_2/H_2O gas equilibria is 843 ± 10 K. Birks (1966) determined the temperature to be 838 ± 10 K by measuring the potential difference between the wustite-iron and the wustite-magnetite buffers. These are in excellent agreement with the other experiments. The final calculated breakdown temperature is 840.2 K.

During the evaluation, the log $f(O_2)$-composition data were used to derive the properties of the defect phase with an iron/oxygen ration of 0.947. Because the properties of the hypothetical end-member "FeO" remain unevaluated, only the thermochemical data for formation from the elements are tabulated.

1.5.5.29. $FeSiO_3$, ferrosilite (formula weight = 131.931 g/mol)

Tables 256 and 257 contain the sources of data used in the final evaluation of the properties of ferrosilite. Other sources, though cited in the reference list, were deleted in preliminary evaluations.

Table 254. Sources of thermophysical data for wustite, $Fe_{.947}O$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	0.0
Hazen and others, 1981	molar volume	X-ray	11	298	1.01-54700	0.00±0.03
Coughlin and others, 1951	heat content	drop cal.	25	341-1614	1.01	0.05±0.47
Todd and Bonnickson, 1951	heat capacity	low-temp. cal.	11	202-296	1.01	-0.08±0.79
Todd and Bonnickson, 1951	entropy	low-temp. cal.	1	298	1.01	1.64

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 255. Sources of thermochemical data for wustite, $Fe_{.947}O$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
CA	Birks, 1966	Electrochemistry	1	838	0.001	-55.492	-265.390
CA	Rau, 1972	Gas reduction	1	843	0.001	-55.747	-265.453
CD	Composite set	Gas reduction	14	1323-1573	0.001	-272.551±0.118	-265.127
CD	Darken and Gurry, 1945	Gas reduction	3	1373-1573	0.001	-272.492±0.137	-265.068
CE	Ackermann & Sanford, 1966	Gas reduction	5	972-1277	0.001	-905.281±0.544	-265.405
CE	Composite set	Gas reduction	12	1373-1573	0.001	-904.952±0.196	-265.295
CE	Darken and Gurry, 1945	Gas reduction	4	1373-1673	0.001	-904.944±0.163	-265.292
CE	Giddings, 1972	Electrochemistry	7	973-1573	0.001	-904.479±0.088	-265.137
CF	Ackermann & Sanford, 1966	Gas reduction	1	1277	0.001	11.462	-264.176
CF	Darken and Gurry, 1945	Gas reduction	8	1311-1638	0.001	10.670±0.219	-264.968
CF	Swaroop and Wagner, 1967	Gas reduction	7	1223-1523	0.001	10.439±0.127	-265.199
CG	Emmett and Schultz, 1933	Gas reduction	19	860-972	0.001	-23.563±0.233	-265.399
CG	Rau, 1972	Gas reduction	11	860-978	0.001	-23.192±0.074	-265.028
CH	Emmett and Schultz, 1933	Gas reduction	17	1080-1172	0.001	275.743±0.202	-265.209
CI	Emmett and Schultz, 1933	Gas reduction	7	1190-1288	0.001	-30.574±0.123	-265.571
CJ	Ackermann & Sanford, 1966	Gas reduction	2	972-1023	0.001	17.265±0.276	-265.797
CK	Ackermann & Sanford, 1966	Gas reduction	2	1075-1182	0.001	317.131±0.499	-265.047
	This Study						-265.416

Reactions:

CA $4\ Fe_{.947}O[\text{wustite}] = Fe_3O_4[\text{magnetite}] + 0.788\ Fe[\text{alpha}]$

CD $Fe_{.947}O[\text{wustite}] = 0.5\ O_2[g] + 0.947\ Fe[\text{gamma}]$

CE $3\ Fe_{.947}O[\text{wustite}] + 0.394\ O_2[g] = 0.947\ Fe_3O_4[\text{magnetite}]$

CF $0.947\ Fe[\text{gamma}] + CO_2[g] = Fe_{.947}O[\text{wustite}] + CO[g]$

CG $0.947\ Fe[\text{alpha}] + H_2O[g] = Fe_{.947}O[\text{wustite}] + H_2[g]$

Table 255. Continued

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
Reactions (continued):							
CH	$0.947\ Fe[alpha\text{-}delta] + H_2O[g] = Fe_{.947}O[wustite] + H_2[g]$						
CI	$0.947\ Fe[gamma] + H_2O[g] = Fe_{.947}O[wustite] + H_2[g]$						
CJ	$0.947\ Fe[alpha] + CO_2[g] = Fe_{.947}O[wustite] + CO[g]$						
CK	$0.947\ Fe[alpha\text{-}delta] + CO_2[g] = Fe_{.947}O[wustite] + CO[g]$						

Table 256. Sources of thermophysical data for ferrosilite, $FeSiO_3$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Burnham, 1966	volume	X-ray	1	298	1.01	0.01
Sueno and others, 1976	volume	X-ray	6	297-1253	1.01	-0.04±0.10

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 257. Sources of thermochemical data for ferrosilite, $FeSiO_3$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
CP	Bohlen and others, 1980	Solid-medium pressure apparatus	8	973-1123	10.5-12.3	-1.253±0.062	-1194.280
CQ	Bohlen and others, 1980	Solid-medium pressure apparatus	8	1173-1323	12.5-15.0	-1.845±0.063	-1194.287
CQ	Navrotsky and others, 1979	Solution calorimetry, borate salt	1	970	0.001	-2.645	-1194.687
CQ	Wood and Kleppa, 1981	Solution calorimetry, borate salt	1	970	0.001	-4.026	-1195.378
	This Study						-1194.286

Reactions:

CP 2 $FeSiO_3$[ferrosilite] = Fe_2SiO_4[fayalite] + SiO_2[quartz, alpha]

CQ 2 $FeSiO_3$[ferrosilite] = Fe_2SiO_4[fayalite] + SiO_2[quartz, beta]

The heat capacity of ferrosilites was estimated using the method described in section 1.3.2, above. The thermochemical properties of ferrosilite were constrained to fit the tightly reversed equilibria between ferrosilite, fayalite, and quartz (Bohlen and others, 1980). These experiments were supported by the borate-salt solution calorimetry.

1.5.5.30. Fe_2O_3, hematite (formula weight = 159.692 g/mol)

Tables 258 and 259 contain the sources of experimental data used to constrain the final evaluation. Below 1000 K the heat capacity experiments of Grønvold and Westrum (1959) and Grønvold and Samuelson (1975) constrained the heat capacity and heat content of hematite. The drop calorimetry of Coughlin and others (1951) were used to contrain the evaluation above 1000 K.

The thermochemical data available in the chemical system Fe-O are all studies on the equilibrium between magnetite and hematite at controlled oxygen fugacities. At the temperature of the experiments, the magnetite phase has a significant solid solution. Activity corrections were made using the formula of Salmon (1961):

$$a^{M}_{Fe_3O_4} = \frac{N^{M}_{Fe_3O_4}}{0.25\, N^{M}_{Fe_2O_3} + N^{M}_{Fe_3O_4}}$$

where the chemical formula denotes the chemical component and the superscript M denotes the phase magnetite. This relationship is in agreement (± 0.01) with the experimental measurements of Darken and Gurry (1946).

Table 258. Sources of thermophysical data for hematite, Fe_2O_3.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	0.0
Willis and Rooksby, 1952	volume	X-ray	2	293-1023	1.01	0.03±0.03
Wilburn and others, 1978	volume	dilatometry	37	293	5300-114000	-0.01±0.17
Lewis and Drickamer, 1966	volume	dilatometry	10	298	1.01-230000	0.78±0.64
Grønvold and Samuelson, 1975	heat capacity	high-temp. cal.	7	973-1054	1.01	-0.07±0.90
Stull and Prophet, 1971	heat capacity	compilation	8	1500-2200	1.01	-0.20±1.34
Grønvold and Samuelson, 1975	heat capacity	high-temp. cal.	63	301-943	1.01	0.09±0.91
Grønvold and Westrum, 1959	heat capacity	low-temp. cal.	19	202-354	1.01	-0.02±0.27
Coughlin and others, 1951	rel. heat content	drop cal.	21	1002-1730	1.01	4.71±11.3
Grønvold and Westrum, 1959	entropy	low-temp. cal.	1	298	1.01	-0.09

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 259. Sources of thermochemical data for hematite, Fe_2O_3.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
CC	Darken and Gurry, 1946	Gas reduction	3	1586-1730	0.001	-167.299±1.011	-827.553
CC	Komarov and others, 1967	Electrochemistry	21	1526-1731	0.001	-166.849±1.078	-827.403
CC	Kurepin, 1975	Electrochemistry	2	1473-1573	0.001	-165.448±0.008	-826.936
CC	Norton, 1955	Mass spectrometry	8	1051-1342	0.001	-161.138±1.124	-825.500
CC	Schmahl, 1941	Gas equilibria	6	1583-1683	0.001	-167.177±0.438	-827.512
CC	Smiltens, 1957	Gas equilibria	4	1452-1731	0.001	-166.769±1.768	-827.377
	This Study						-827.148

Reactions:

CC $2\ Fe_3O_4$[magnetite] + $0.5\ O_2$[g] = $3\ Fe_2O_3$[hematite]

Darken and Gurry (1946), Salmon (1961), and Komarov and others (1967) have shown that the solid solution of Fe_3O_4 in hematite is minor and can be neglected.

Rau (1972) studied the equilibria between hematite and magnetite at 1.01 bars between 767 and 840 K using the gas equilibria between H_2 and H_2O to control the chemical activity of oxygen. The mixture of magnetite + hematite was synthesized from an alpha-FeOOH precipitate by hydrogen reduction near 600 K. The magnetite in the mixture probably contained a significant Fe_2O_3 component and was metastable. The departure of these data from the refinement is consistent with such a hypothesis.

1.5.5.31. Fe_2SiO_4, fayalite (formula weight = 203.777 g/mol)

Tables 260 and 261 contain the sources of data used in the final evaluation of the properties of fayalite. Other data, though cited in the reference list, were deleted in preliminary evaluations.

The thermochemical data of Hewitt (1978) and of Meyer (1981, unpub.) constrain the properties of fayalite. The experimental investigations on the equilibria between fayalite, iron, oxygen (controlled by CO/CO_2 or H_2/H_2O gas equilibria) and an undefined polymorph in the SiO_2 system were given minor weighting because of the lack of positive identification of the SiO_2 polymorph present during the experiment. Where used, the analyses were completed assuming that beta cristobalite was the phase present. This was chosen because of the high temperature and because it readily forms. It is recognized that some interpretations of the data on the stability of the SiO_2

Table 260. Sources of thermophysical data for fayalite, Fe_2SiO_4.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Hazen, 1977	volume	X-ray	3	296	1.01-42000	0.03±0.09
Hazen, 1977	volume	X-ray	3	77-296	1.01	0.26±0.11
Smyth, 1975	volume	X-ray	6	293-1173	1.01	-0.01±0.14
Robie and Hemingway, 1982(unpub.)	heat capacity	low-temp. cal.	31	208-381	1.01	0.01±0.09
Orr, 1953	heat content	drop cal.	13	395-1370	1.01	-0.23±0.50
Robie and Hemingway, 1982(unpub.)	entropy	low-temp. cal.	1	298	1.01	-0.36

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 261. Sources of thermochemical data for fayalite, Fe_2SiO_4.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
CL	Hewitt, 1978	Gas reduction	8	923-1128	1.0	704.020±0.808	-1478.538
CM	Meyer, J., 1981(unpub.)	Gas-medium pressure apparatus	7	922-1046	0.001	1888.729±1.693	-1479.897
CN	Lebedev & Lefitskii, 1962	Gas reduction	4	1123-1173	0.001	-311.995±0.171	-1479.394
CO	Lebedev & Lefitskii, 1962	Gas reduction	13	1223-1423	0.001	12.555±0.352	-1477.688
CO	Schwerdtfeger & Muan, 1966	Gas reduction	3	1273-1473	0.001	12.050±0.184	-1478.698
CP	Bohlen and others, 1980	Solid-medium pressure apparatus	8	973-1123	10.5-12.3	-1.253±0.062	-1479.155
CQ	Bohlen and others, 1980	Solid-medium pressure apparatus	8	1173-1323	12.5-15.0	-1.845±0.063	-1479.170
CQ	Navrotsky and others, 1979	Solution calorimetry, borate salt	1	970	0.001	-2.645	-1479.970
CQ	Wood and Kleppa, 1981	Solution calorimetry, borate salt	1	970	0.001	-4.026	-1481.351
	This Study						-1479.168

Reactions:

CL Fe_3O_4[magnetite] + 1.5 SiO_2[quartz, beta] + H_2[g] = 1.5 Fe_2SiO_4[fayalite] + H_2O[g]

CM 2 Fe_3O_4[magnetite] + 3 SiO_2[quartz, beta] = 3 Fe_2SiO_4[fayalite] + O_2[g]

CN 0.5 Fe_2SiO_4[fayalite] + CO[g] = Fe[alpha-delta] + 0.5 SiO_2[cristobalite] + CO_2[g]

CO 0.5 Fe_2SiO_4[fayalite] + CO[g] = Fe[gamma] + 0.5 SiO_2[cristobalite] + CO_2[g]

CP 2 $FeSiO_3$[ferrosilite] = Fe_2SiO_4[fayalite] + SiO_2[quartz, alpha]

CQ 2 $FeSiO_3$[ferrosilite] = Fe_2SiO_4[fayalite] + SiO_2[quartz, beta]

polymorphs would make tridymite the stable phase under the experimental environment.

1.5.5.32. Fe_3O_4, magnetite (formula weight = 231.539 g/mol)

The sources of data used in the final evaluation are given on tables 262 and 263. Other data, though cited in the reference list, were deleted prior to the final evaluation.

The heat capacity at temperatures below 1000 K were dependent primarily on the experimentally measured heat capacities by Westrum and Grønvold (1965) and by Grønvold and Sveen (1974). The drop calorimetry of Coughlin and others (1951) were so weighted as to constrain the fit above 1000 K only. The thermochemical properties observed over the range 583 to 1731 K are consistent with $S\beta$ = zero. No allowance of an additional contribution due to disorder of any type is needed. With the exception of the relatively inaccurate data of Norton (1955), the final solution of the properties is consistent with the tabulated sources.

1.5.5.33. H_2, hydrogen (ideal gas, formula weight = 2.016 g/mol)

The properties of the ideal diatomic gas were taken from the JANAF Thermochemical Tables[a]. The volumetric properties were not needed in this study and therefore not evaluated.

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[a]JANAF Thermochemical Tables, looseleaf pages for 1977 issued by Dow Chemical Company, 1707 Building, Midland, Michigan.

Table 262. Sources of thermophysical data for magnetite, Fe_3O_4.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	0.0
Tombs and Rooksby, 1951	volume	X-ray	2	165-295	1.01	0.0±0.0
Wilburn and Bassett, 1977	volume	dilatometry	10	293	1.01-65000	0.02±0.17
Stull and Prophet, 1971	heat capacity	compilation	6	1700-2200	1.01	0.11±0.95
Grønvold and Sveen, 1974	heat capacity	high-temp. cal.	17	861-1044	1.01	0.20±1.76
Grønvold and Sveen, 1974	heat capacity	high-temp. cal.	59	299-837	1.01	0.44±1.48
Westrum and Grønvold, 1965	heat capacity	low-temp. cal.	16	202-347	1.01	-0.05±0.21
Coughlin and others, 1951	heat content	drop cal.	19	874-1825	1.01	-2.8±6.0
Westrum and Grønvold, 1965	entropy	low-temp. cal.	1	298	1.01	0.09

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 263. Sources of thermochemical data for magnetite, Fe_3O_4.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
CA	Birks, 1966	Electrochemistry	1	838	0.001	-55.492	-1117.156
CA	Rau, 1972	Gas reduction	1	843	0.001	-55.747	-1117.411
CB	Emmett and Schultz, 1933	Gas reduction	35	674-823	0.001	37.696±0.165	-1116.398
CB	Rau, 1972	Gas reduction	17	583-810	0.001	37.051±0.244	-1118.978
CC	Darken and Gurry, 1946	Gas reduction	3	1586-1730	0.001	-167.299±1.011	-1117.870
CC	Komarov and others, 1967	Electrochemistry	21	1526-1731	0.001	-166.849±1.078	-1117.645
CC	Kurepin, 1975	Electrochemistry	2	1473-1573	0.001	-165.448±0.008	-1116.945
CC	Norton, 1955	Mass spectrometry	8	1051-1342	0.001	-161.138±1.124	-1114.790
CC	Schmahl, 1941	Gas equilibria	6	1583-1683	0.001	-167.177±0.438	-1117.809
CC	Smiltens, 1957	Gas equilibria	4	1452-1731	0.001	-166.769±1.768	-1117.605
CL	Ackermann & Sanford, 1966	Gas reduction	5	972-1277	0.001	-905.281±0.544	-1117.226
CE	Composite set	Gas reduction	12	1373-1573	0.001	-904.952±0.196	-1116.879
CE	Darken and Gurry, 1945	Gas reduction	4	1373-1673	0.001	-904.944±0.163	-1116.870
CE	Giddings, 1972	Electrochemistry	7	973-1573	0.001	-904.479±0.088	-1116.379
CL	Hewitt, 1978	Gas reduction	8	923-1128	1.0	704.020±0.808	-1116.318
CM	Meyer, J., 1981(unpub.)	Gas-medium pressure apparatus	7	922-1046	0.001	1888.729±1.693	-1117.809
	This Study						-1117.262

Reactions:

CA $4\ Fe_{.947}O[\text{wustite}] = Fe_3O_4[\text{magnetite}] + 0.788\ Fe[\text{alpha}]$

CB $0.25\ Fe_3O_4[\text{magnetite}] + H_2[g] = 0.75\ Fe[\text{alpha}] + H_2O[g]$

CC $2\ Fe_3O_4[\text{magnetite}] + 0.5\ O_2[g] = 3\ Fe_2O_3[\text{hematite}]$

CE $3\ Fe_{.947}O[\text{wustite}] + 0.394\ O_2[g] = 0.947\ Fe_3O_4[\text{magnetite}]$

CL $Fe_3O_4[\text{magnetite}] + 1.5\ SiO_2[\text{quartz, beta}] + H_2[g] = 1.5\ Fe_2SiO_4[\text{fayalite}] + H_2O[g]$

CM $2\ Fe_3O_4[\text{magnetite}] + 3\ SiO_2[\text{quartz, beta}] = 3\ Fe_2SiO_4[\text{fayalite}] + O_2[g]$

1.5.5.34. H_2O, water and the ideal and real gases (formula weight = 18.0152 g/mol)

The entropy and Gibbs energy of formation at 298.15 K were taken from the CODATA Task Group (1978). The other properties for the ideal gas and for water and the real gas were taken from the work of Haar and others (1979, 1981).

1.5.5.35. H_4SiO_4, silicic acid (formula weight = 96.115 g/mol)

Hemley and others (1977a, 1980) measured the silica concentration in the aqueous fluid coexisting with quartz at 1 and 2 kb. From these data we obtained the following expression for the "Gibbs energy" for the reaction $SiO_2(quartz,T,P_r) + H_2O(gas,T,P_r) = H_4SiO_4(aqueous, T,P_r)$:

$$\Delta G_{r_{T,P_r}} = -\frac{a_{1,j}}{2T} + 4\,a_{2,j}\sqrt{T} + a_{3,j}\,(T - T\ln T) - a_{4,j}\,T + a_{5,j} - a_{6,j}\,T^2 + a_{7,j}\,\frac{T^3}{6} \qquad (28)$$

In the above equation, T is the absolute temperature in kelvins and the constants $a_{i,j}$ are as follows:

i	(i,P_r=1 kb)	(i,P_r=2 kb)
1	2.62154×10^{5}	$2.62154\times10_{5}$
2	5.48272×10^{3}	4.97309×10^{3}
3	-1.04134×10^{2}	-1.04134×10^{2}
4	9.79088×10^{2}	9.39015×10^{2}

i	$(i,P_r=1\ kb)$	$(i,P_r=2\ kb)$
5	-2.28273×10^{5}	-1.97113×10^{5}
6	-3.69344×10^{-2}	-3.69344×10^{-2}
7	8.93770×10^{-6}	8.93770×10^{-6}

In deriving this relation, it is assumed that the activity coefficient of the silicic acid species is constant in the dilute aqueous solutions and can be neglected.

In the experiments in the magnesia-silica-water system (Hemley and others, 1977a) and in the alumina-silica-water system (Hemley and others, 1980), the concentrations of aqueous silicic acid coexisting with mineral pairs were measured at 1 and 2 kb. These data were evaluated by using the above relations for the formation of aqueous silicic acid from 1-atm quartz and 1-atm H_2O[g].

1.5.5.36. Mg, magnesium (formula weight = 24.305 g/mol)

The properties of magnesium polymorphs were taken from the compilation of Hultgren and others (1973). The volumetric properties were not needed in this study and were not evaluated.

1.5.5.37. $MgCO_3$, magnesite (formula weight = 84.314 g/mol)

Tables 264 and 265 contain the sources of data used in the final evaluation. There exists a large body of information in which the gas phase contained both H_2O[g] and CO_2[g]. Those data could not be used to identify the properties of magnesite and the magnesium silicates better because the mixing properties of the two gaseous species would

Table 264. Sources of thermophysical data for magnesite, $MgCO_3$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298	1.01	
Hemingway and others, 1977	heat capacity	low-T. cal.	29	207-384	1.01	0.047±0.182
Anderson, 1934	heat capacity	low-T. cal.	5	201-292	1.01	0.413±0.531
Kelley, 1960	rel. enthalpy	drop cal.	4	400-700	1.01	0.845±0.471
Robie and others, 1979	heat capacity	compilation	6	298-600	1.01	0.728±0.423
Robie and others, 1979	entropy	compilation	1	298	1.01	0.014

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 265. Sources of thermochemical data for magnesite, $MgCO_3$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
DB	Johannes, 1969	Gas-medium pressure apparatus	1 pr	828-833	2.0	90.972±0.242	-1113.810
DC	Harker and Tuttle, 1955	Decomposition pressure	5	872-1123	0.06-2.1	119.601±1.191	-1112.894
DC	Irving and Wyllie, 1975	Solid-medium pressure apparatus	4	1623-1743	17.0-20.0	116.347±1.769	-1115.237
DC	Johannes and Metz, 1968	Gas-medium pressure apparatus	2 pr	973-1043	0.5-1.0	117.479±0.537	-1114.105
DC	Marc and Sinek, 1913	Decomposition pressure	24	671-782	0.0008-0.011	118.751±1.082	-1112.834
	This Study						-1113.225

Reactions:

DB $MgCO_3$[magnesite] + $MgSiO_3$[enstatite] = Mg_2SiO_4[forsterite] + CO_2[g]

DC $MgCO_3$[magnesite] = MgO[periclase] + CO_2[g]

only introduce larger uncertainties. The accepted data are in good agreement.

1.5.5.38. MgO, periclase (formula weight = 40.304 g/mol)

The thermodynamic properties for periclase were taken from the JANAF Thermochemical Tables[a]. The volumetric properties were evaluated from the sources cited on table 266.

1.5.5.39. $Mg(OH)_2$, brucite (formula weight = 58.320 g/mol)

The tables 267 and 268 contain the sources of data used in this evaluation. Other data, though cited in the reference list, were deleted prior to the final evaluation.

1.5.5.40. $MgSiO_3$, clinoenstatite, enstatite, and protoenstatite (formula weight = 100.389 g/mol)

The sources of data used to evaluate the properties of the pyroxene polymorphs clinoenstatite, enstatite, and protoenstatite are contained in tables 269 through 274. Other data, though cited in the reference list, were deleted prior to the final evaluation.

The fitted inversions at 1.01 bars are as follows:

Equilibrium	Temperature
clinoenstatite = enstatite	968.5 K
enstatite = protoenstatite	1257.4 K

The phase equilibria cited on tables 270, 272 and 274 are very consistent with the final results of the evaluation.

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[a]JANAF Thermochemical Tables, looseleaf pages for 1978 issued by Dow Chemical Company, 1707 Building, Midland, Michigan.

Table 266. Sources of thermophysical data for periclase, MgO.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Hazen, 1976a	volume	X-ray	15	77-1315	1-24000	0.002±0.090
Skinner, 1957	volume	X-ray	12	284-976	1.01	0.007±0.057
Robie and others, 1979	volume	compilation	1	298	1.01	0.035

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 267. Sources of thermophysical data for brucite, $Mg(OH)_2$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Robie and others, 1979	volume	compilation	1	298		
Giauque and Archibald, 1937	heat capacity	low-T. cal.	21	217-321	1.01	0.219±0.631
King and others, 1975	rel. enthalpy	drop cal.	12	350-699	1.01	0.219±0.332
Giauque and Archiblad, 1937	entropy	low-T. cal.	1	298	1.01	0.0037

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 268. Sources of thermochemical data for brucite, $Mg(OH)_2$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
DA	Barnes and Ernst, 1963	Gas-medium pressure apparatus	16	817-937	0.2-2.0	82.940±0.758	-924.600
DA	Fyfe and Godwin, 1962	Gas-medium pressure apparatus	1 pr	864-893	1.0	82.324±0.893	-925.215
DA	Fyfe, 1958	Decomposition pressure	10 pr	803-843	0.2-0.7	82.045±0.913	-925.494
DA	Kennedy, 1956	Decomposition pressure	10 pr	773-873	0.1-1.1	81.663±1.438	-925.877
DA	Schramke and others, 1982	Gas-medium pressure apparatus	4 pr	963-1079	3.9-8.1	82.125±0.592	-925.415
DI	Johannes, 1968	Gas-medium pressure apparatus	7 pr	603-713	0.5-7.0	216.829±2.644	-922.584
	This Study						-925.307

Reactions:

DA $Mg(OH)_2$[brucite] = MgO[periclase] + H_2O[g]

DI $Mg_3Si_2O_5(OH)_4$[chrysotile] + $Mg(OH)_2$[brucite] = 2 Mg_2SiO_4[forsterite] + 3 H_2O[g]

Table 269. Sources of thermophysical data for clinoenstatite, $MgSiO_3$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Evans, Howard, 1977(unpub.)	volume	X-ray	7	298-973	1.01	0.041±0.148
Stephenson and others, 1966	volume	X-ray	3	298	1.01	0.006±0.012
Kelley, 1943	heat capacity	low-T. cal.	9	216-295	1.01	0.035±0.311
Wagner, 1932	rel. enthalpy	drop cal.	4	580-767	1.01	0.362±0.631
Wagner, 1932	rel. enthalpy	drop cal.	5	966-1177	1.01	0.518±0.345
Robie and others, 1979	heat capacity	compilation	14	298-1600	1.01	0.018±0.638
Robie and others, 1979	entropy	compilation	1	298	1.01	0.147

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 270. Sources of thermochemical data for clinoenstatite, $MgSiO_3$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H_r°(298.15 K) Third Law, kJ	H_f°(298.15 K) kJ/mol
DJ	Boyd and England, 1965	Solid-medium pressure apparatus	4 pr	893-1033	5.0-40.0	-0.142±0.120	-1544.834
DL	Greenwood, 1963	Gas-medium pressure apparatus	1 pr	935-985	2.0-2.6	102.495±1.674	-1544.746
DQ	Charlu and others, 1975	Solution calorimetry, borate salt	1	970	0.001	32.720	-1153.906
DQ	Kiseleva and others, 1981	Solution calorimetry, borate salt	1	1170	0.001	30.672	-1155.954
	This Study						-1544.844

Reactions:

DJ $MgSiO_3$[enstatite] = $MgSiO_3$[clinoenstatite]

DL Mg_2SiO_4[forsterite] + $Mg_3Si_4O_{10}(OH)_2$[talc] = 5 $MgSiO_3$[clinoenstatite] + H_2O[g]

DQ $MgSiO_3$[clinoenstatite] = MgO[periclase] + SiO_2[quartz, beta]

Table 271. Sources of thermophysical data for orthoenstatite, $MgSiO_3$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Ralph and others, 1981	volume	X-ray	23	296-773	1-40200	0.016±0.181
Ralph and Ghose, 1980	volume	X-ray	2	298	1-21000	0.044±0.056
Evans, Howard, 1977(unpub.)	volume	X-ray	6	298-1073	1.01	0.032±0.054
Charlu and others, 1975	volume	X-ray	2	298	1.01	0.077±0.077
Chernosky and Autio, 1979	volume	X-ray	1	298	1.01	0.009
Krupka and others, 1980	heat capacity	d.s.c.	151	200-1000	1.01	0.012±0.472
Krupka and others, 1980	entropy	low-T. cal.	1	298	1.01	0.008

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 272. Sources of thermochemical data for enstatite, $MgSiO_3$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
DB	Johannes, 1969	Gas-medium pressure apparatus	1 pr	828-833	2.0	90.972±0.242	-1545.281
DF	Greenwood, 1963	Gas-medium pressure apparatus	1 pr	968-984	2.0	87.806±0.471	-1544.610
DF	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	936-950	1.0	87.967±0.475	-1544.592
DG	Chernosky and Autio, 1979	Gas-medium pressure apparatus	4 pr	937-1048	0.5-3.0	93.681±1.030	-1544.519
DG	Greenwood, 1963	Gas-medium pressure apparatus	2 pr	1023-1048	2.0-2.6	92.088±0.854	-1544.746
DG	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	992-1012	1.0	93.708±0.699	-1544.514
DJ	Boyd and England, 1965	Solid-medium pressure apparatus	4 pr	893-1033	5.0-40.0	-0.142±0.120	-1544.686
DK	Atlas, 1952	Rapid quench	1 pr	1248-1268	0.001	12.811±0.189	-1544.690
DK	Boyd and others, 1964	Solid-medium pressure apparatus	1 pr	1823	6.1-7.4	12.805±0.061	-1544.696
DM	Chernosky, 1976	Gas-medium pressure apparatus	3 pr	921-1017	0.5-2.0	107.174±2.117	-1544.774
DM	Chernosky, 1976	Gas-medium pressure apparatus	8 pr	928-1073	0.5-10.0	107.313±1.824	-1544.728
DM	Greenwood, 1963	Gas-medium pressure apparatus	1 pr	976-1048	2.0-2.6	107.717±2.378	-1544.593
DM	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	955-971	1.0	106.956±0.726	-1544.847
DO	Chernosky, 1976	Gas-medium pressure apparatus	1 pr	873-894	0.5	101.268±0.892	-1544.839
	This Study						-1544.696

Reactions:

DB $MgCO_3$[magnesite] + $MgSiO_3$[enstatite] = Mg_2SiO_4[forsterite] + CO_2[g]

DF $Mg_7Si_8O_{22}(OH)_2$[anthophyllite] + 4 Mg_2SiO_4[forsterite] = 9 $MgSiO_3$[enstatite] + H_2O[g]

DG $Mg_7Si_8O_{22}(OH)_2$[anthophyllite] = 7 $MgSiO_3$[enstatite] + SiO_2[quartz] + H_2O[g]

DJ $MgSiO_3$[enstatite] = $MgSiO_3$[clinoenstatite]

DK $MgSiO_3$[enstatite] = $MgSiO_3$[protoenstatite]

DM $Mg_3Si_4O_{10}(OH)_2$[talc] = 3 $MgSiO_3$[enstatite] + SiO_2[quartz] + H_2O[g]

DO Mg_2SiO_4[forsterite] + $Mg_3Si_4O_{10}(OH)_2$[talc] = 5 $MgSiO_3$[enstatite] + H_2O[g]

Table 273. Sources of thermophysical data for protoenstatite, $MgSiO_3$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Evans, Howard, 1977(unpub.)	volume	X-ray	9	373-1473	1.01	0.013±0.083
Smith, 1959	volume	X-ray	1	298	1.01	0.117
Wagner, 1932	rel. enthalpy	drop cal.	4	1364-1570	1.01	-5.2±0.5

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 274. Sources of thermochemical data for protoenstatite, $MgSiO_3$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
DK	Atlas, 1952	Rapid quench	1 pr	1248-1268	0.001	12.811±0.189	-1531.879
DK	Boyd and others, 1964	Solid-medium pressure apparatus	1 pr	1823	6.1-7.4	12.805±0.061	-1531.885
	This Study						-1531.885

Reactions:

DK $MgSiO_3$[enstatite] = $MgSiO_3$[protoenstatite]

1.5.5.41. Mg_2SiO_4, forsterite (formula weight = 140.693 g/mol)

The sources of data used in the final evaluation are contained on tables 275 and 276. Other data listed in the reference list were deleted prior to the final evaluation. The data used are in satisfactory agreement.

1.5.5.42. $Mg_3Si_2O_5(OH)_4$, chrysotile (formula weight = 277.112 g/mol)

Tables 277 and 278 contain the sources of data used to evaluate the properties of the serpentine mineral, chrysotile. On table 278 the enthalpy of formation from the elements appears to be incorrect, that is, more negative than any of the "averages" shown. The final solution was assymetrically to one side of the measured brackets. The weighted solution is consistent with the experimental data.

1.5.5.43. $Mg_3Si_4O_{10}(OH)_2$, talc (formula weight = 379.266 g/mol)

Tables 279 and 280 contain the sources of data used in the final evaluation. All other data, though cited in the reference list, were dropped prior to the final fitting.

1.5.5.44. $Mg_7Si_8O_{22}(OH)_2$, anthophyllite (formula weight = 780.820 g/mol)

Tables 281 and 282 contain the sources of data used in the evaluation. All other data, though cited in the reference list, were deleted prior to the final evaluation. The collected data are in good internal agreement.

Table 275. Sources of thermophysical data for forsterite, Mg_2SiO_4.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Olinger and Halleck, 1974	volume ratio	X-ray	7	298	1-108500	0.079±0.186
Hazen, 1976b	volume	X-ray	4	273	1-50000	0.004±0.095
Hazen, 1976b	volume	X-ray	14	77-1293	1.01	0.176±0.115
Skinner, 1962	volume	X-ray	15	298-1400	1.01	0.270±0.047
Charlu and others, 1975	volume	X-ray	1	298	1.01	0.024
Kelley, 1943	heat capacity	low-T. cal.	9	216-295	1.01	0.005±0.243
Orr, 1953	rel. enthalpy	drop cal.	16	398-1808	1.01	0.142±0.344
Robie and others, 1979	entropy	compilation	1	298	1.01	0.337

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 276. Sources of thermochemical data for forsterite, Mg_2SiO_4.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
DB	Johannes, 1969	Gas-medium pressure apparatus	1 pr	828-833	2.0	90.972±0.242	-2173.314
DD	Greenwood, 1963	Gas-medium pressure apparatus	3 pr	936-965	1.0-4.0	486.883±3.170	-2171.724
DD	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	902-916	1.0	475.780±3.247	-2174.500
DF	Greenwood, 1963	Gas-medium pressure apparatus	1 pr	968-984	2.0	87.806±0.471	-2171.956
DF	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	936-950	1.0	87.967±0.475	-2171.795
DH	Evans and others, 1976	Gas- & solid-medium pressure apparatus	5 pr	753-933	2.0-15.0	2168.159±30.183	-2173.394
DH	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	775-799	1.0	2201.949±21.067	-2171.517
DI	Johannes, 1968	Gas-medium pressure apparatus	7 pr	603-713	0.5-7.0	216.829±2.644	-2171.367
DL	Chernosky, 1976	Gas-medium pressure apparatus	5 pr	923-979	1.0-6.0	101.574±0.869	-2173.157
DL	Greenwood, 1963	Gas-medium pressure apparatus	1 pr	935-985	2.0-2.6	102.495±1.674	-2172.237
DL	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	908-924	1.0	101.086±0.710	-2173.646
DN	Chernosky, 1982	Gas-medium pressure apparatus	5 pr	672-809	0.5-6.9	695.118±9.175	-2172.105
DN	Hemley and others, 1977a	H_4SiO_4 concentration	1 pr	708-720	1.0	698.480±3.379	-2171.544
DO	Chernosky, 1976	Gas-medium pressure apparatus	1 pr	873-894	0.5	101.268±0.892	-2172.706
DP	Charlu and others, 1975	Solution calorimetry, borate salt	1	970	0.001	59.502	-2171.655
DP	Kiseleva and others, 1981	Solution calorimetry, borate salt	1	1170	0.001	57.179	-2173.978
	This Study						-2172.729

Reactions:

DB $MgCO_3$[magnesite] + $MgSiO_3$[enstatite] = Mg_2SiO_4[forsterite] + CO_2[g]

DD 4 Mg_2SiO_4[forsterite] + 9 $Mg_3Si_4O_{10}(OH)_2$[talc] = 5 $Mg_7Si_8O_{22}(OH)_2$[anthophyllite] + 4 H_2O[g]

DF $Mg_7Si_8O_{22}(OH)_2$[anthophyllite] + 4 Mg_2SiO_4[forsterite] = 9 $MgSiO_3$[enstatite] + H_2O[g]

DH $Mg_{48}Si_{34}O_{85}(OH)_{62}$[antigorite] = 18 Mg_2SiO_4[forsterite] + 4 $Mg_3Si_4O_{10}(OH)_2$[talc] + 27 H_2O[g]

DI $Mg_3Si_2O_5(OH)_4$[chrysotile] + $Mg(OH)_2$[brucite] = 2 Mg_2SiO_4[forsterite] + 3 H_2O[g]

DL Mg_2SiO_4[forsterite] + $Mg_3Si_4O_{10}(OH)_2$[talc] = 5 $MgSiO_3$[clinoenstatite] + H_2O[g]

Table 27b. Continued

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H_r°(298.15 K) Third Law, kJ	H_f°(298.15 K) kJ/mol
Reactions (continued):							
DN	$5\ Mg_3Si_2O_5(OH)_4$[chrysotile] = $6\ Mg_2SiO_4$[forsterite] + $Mg_3Si_4O_{10}(OH)_2$[talc] + $9\ H_2O$[g]						
DO	Mg_2SiO_4[forsterite] + $Mg_3Si_4O_{10}(OH)_2$[talc] = $5\ MgSiO_3$[enstatite] + H_2O[g]						
DP	Mg_2SiO_4[forsterite] = $2\ MgO$[periclase] + SiO_2[quartz, beta]						

Table 277. Sources of thermophysical data for chrysotile, $Mg_3Si_2O_5(OH)_4$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Hemley and others, 1977a	volume	X-ray	1	298	1.01	0.053
King and others, 1967	heat capacity	low-T. cal.	10	206-296	1.01	0.002±0.072
King and others, 1967	entropy	low-T. cal.	1	298	1.01	0.004

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 278. Sources of thermochemical data for chrysotile, $Mg_3Si_2O_5(OH)_4$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Pressure (kb)	H_r°(298.15 K) Third Law, kJ	H_f°(298.15 K) kJ/mol
DI	Johannes, 1968	Gas-medium pressure apparatus	7 pr	603-713	0.5-7.0	216.829±2.644	-4479.314
DN	Chernosky, 1982	Gas-medium pressure apparatus	5 pr	672-809	0.5-6.9	695.118±9.175	-4481.287
DN	Hemley and others, 1977a	H_4SiO_4 concentration	1 pr	708-720	1.0	698.480±3.379	-4480.615
	This Study						-4482.037

Reactions:

DI $Mg_3Si_2O_5(OH)_4$[chrysotile] + $Mg(OH)_2$[brucite] = 2 Mg_2SiO_4[forsterite] + 3 H_2O[g]

DN 5 $Mg_3Si_2O_5(OH)_4$[chrysotile] = 6 Mg_2SiO_4[forsterite] + $Mg_3Si_4O_{10}(OH)_2$[talc] + 9 H_2O[g]

Table 279. Sources of thermophysical data for talc, $Mg_3Si_4O_{10}(OH)_2$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Vaidya and others, 1973	volume ratio	rel. volume	9	298	5000-45000	0.020±0.062
Hemley and others, 1977a	volume	X-ray	1	298	1.01	0.707
Robie and Stout, 1963	heat capacity	low-T. cal.	9	240-298	1.01	0.323±0.481
Robie and others, 1979	heat capacity	compilation	3	298-500	1.01	0.487±1.018
Krupka and others, 1977	heat capacity	d.s.c.	15	298-650	1.01	0.582±0.772
Krupka and others, 1977	entropy	low-T. cal.	1	298	1.01	0.0005

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 280. Sources of thermochemical data for talc, $Mg_3Si_4O_{10}(OH)_2$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Pressure (kb)	H_r°(298.15 K) Third Law, kJ	H_f°(298.15 K kJ/mol
DD	Greenwood, 1963	Gas-medium pressure apparatus	3 pr	936-965	1.0-4.0	486.883±3.170	-6199.77
DD	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	902-916	1.0	475.780±3.247	-6201.00
DE	Chernosky and Autio, 1979	Gas-medium pressure apparatus	5 pr	920-1015	0.5-3.0	473.811±5.074	-6200.32
DE	Greenwood, 1963	Gas-medium pressure apparatus	1 pr	967-984	2.0	470.118±3.337	-6200.85
DE	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	941-955	1.0	469.296±2.991	-6200.96
DH	Evans and others, 1976	Gas- & solid-medium pressure apparatus	5 pr	753-933	2.0-15.0	2168.159±30.183	-6203.21
DH	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	775-799	1.0	2201.949±21.067	-6194.76
DL	Chernosky, 1976	Gas-medium pressure apparatus	5 pr	923-979	1.0-6.0	101.574±0.869	-6200.64
DL	Greenwood, 1963	Gas-medium pressure apparatus	1 pr	935-985	2.0-2.6	102.495±1.674	-6199.72
DL	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	908-924	1.0	101.086±0.710	-6201.13
DM	Chernosky, 1976	Gas-medium pressure apparatus	3 pr	921-1017	0.5-2.0	107.174±2.117	-6200.45
DM	Chernosky, 1976	Gas-medium pressure apparatus	8 pr	928-1073	0.5-10.0	107.313±1.824	-6200.31
DM	Greenwood, 1963	Gas-medium pressure apparatus	1 pr	976-1048	2.0-2.6	107.717±2.378	-6199.91
DM	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	955-971	1.0	106.956±0.726	-6200.67
DN	Chernosky, 1982	Gas-medium pressure apparatus	5 pr	672-809	0.5-6.9	695.118±9.175	-6196.47
DN	Hemley and others, 1977a	H_4SiO_4 concentration	1 pr	708-720	1.0	698.480±3.379	-6193.10
DO	Chernosky, 1976	Gas-medium pressure apparatus	1 pr	873-894	0.5	101.268±0.892	-6200.19
	This Study						-6200.21

Reactions:

DD $4\ Mg_2SiO_4[forsterite] + 9\ Mg_3Si_4O_{10}(OH)_2[talc] = 5\ Mg_7Si_8O_{22}(OH)_2[anthophyllite] + 4\ H_2O[g]$

DE $7\ Mg_3Si_4O_{10}(OH)_2[talc] = 3\ Mg_7Si_8O_{22}(OH)_2[anthophyllite] + 4\ SiO_2[quartz] + 4\ H_2O[g]$

DH $Mg_{48}Si_{34}O_{85}(OH)_{62}[antigorite] = 18\ Mg_2SiO_4[forsterite] + 4\ Mg_3Si_4O_{10}(OH)_2[talc] + 27\ H_2O[g]$

DL $Mg_2SiO_4[forsterite] + Mg_3Si_4O_{10}(OH)_2[talc] = 5\ MgSiO_3[clinoenstatite] + H_2O[g]$

DM $Mg_3Si_4O_{10}(OH)_2[talc] = 3\ MgSiO_3[enstatite] + SiO_2[quartz] + H_2O[g]$

Table 280. Continued

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_f(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
Reactions (continued):							
DN	$5\ Mg_3Si_2O_5(OH)_4$[chrysotile] = $6\ Mg_2SiO_4$[forsterite] + $Mg_3Si_4O_{10}(OH)_2$[talc] + $9\ H_2O$[g]						
DO	Mg_2SiO_4[forsterite] + $Mg_3Si_4O_{10}(OH)_2$[talc] = $5\ MgSiO_3$[enstatite] + H_2O[g]						

Table 281. Sources of thermophysical data for anthophyllite, $Mg_7Si_8O_{22}(OH)_2$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Chernosky and Autio, 1979	volume	X-ray	1	298	1.01	0.266
Krupka, Kenneth M., 1982(unpub.)	heat capacity	d.s.c.	36	200-700	1.01	0.008±0.135
Krupka, Kenneth M., 1982(unpub.)	entropy	low-T. cal.	1	298	1.01	0.008

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 282. Sources of thermochemical data for anthophyllite, $Mg_7Si_8O_{22}(OH)_2$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Pressure (kb)	H°_r(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
DD	Greenwood, 1963	Gas-medium pressure apparatus	3 pr	936-965	1.0-4.0	486.883±3.170	-12057.562
DD	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	902-916	1.0	475.780±3.247	-12059.783
DE	Chernosky and Autio, 1979	Gas-medium pressure apparatus	5 pr	920-1015	0.5-3.0	473.811±5.074	-12058.612
DE	Greenwood, 1963	Gas-medium pressure apparatus	1 pr	967-984	2.0	470.118±3.337	-12059.843
DE	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	941-955	1.0	469.296±2.991	-12060.117
DF	Greenwood, 1963	Gas-medium pressure apparatus	1 pr	968-984	2.0	87.806±0.471	-12057.593
DF	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	936-950	1.0	87.967±0.475	-12057.432
DG	Chernosky and Autio, 1979	Gas-medium pressure apparatus	4 pr	937-1048	0.5-3.0	93.681±1.030	-12057.124
DG	Greenwood, 1963	Gas-medium pressure apparatus	2 pr	1023-1048	2.0-2.6	92.088±0.854	-12058.717
DG	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	992-1012	1.0	93.708±0.699	-12057.097
	This Study						-12058.366

Reactions:

DD $4\ Mg_2SiO_4$[forsterite] + $9\ Mg_3Si_4O_{10}(OH)_2$[talc] = $5\ Mg_7Si_8O_{22}(OH)_2$[anthophyllite] + $4\ H_2O$[g]

DE $7\ Mg_3Si_4O_{10}(OH)_2$[talc] = $3\ Mg_7Si_8O_{22}(OH)_2$[anthophyllite] + $4\ SiO_2$[quartz] + $4\ H_2O$[g]

DF $Mg_7Si_8O_{22}(OH)_2$[anthophyllite] + $4\ Mg_2SiO_4$[forsterite] = $9\ MgSiO_3$[enstatite] + H_2O[g]

DG $Mg_7Si_8O_{22}(OH)_2$[anthophyllite] = $7\ MgSiO_3$[enstatite] + SiO_2[quartz] + H_2O[g]

1.5.5.45. $Mg_{48}Si_{34}O_{85}(OH)_{62}$, antigorite (formula weight = 4535.949 g/mol)

Tables 283 and 284 contain the sources of data used in the final evaluation. Other data that were considered but not used are given in the reference list. The thermochemical data, cited in table 284, appear to be inconsistent. However, when the size of the chemical formula for one mole is considered, the two sets are acceptably consistent.

1.5.5.46. O_2, oxygen (ideal gas, formula weight = 31.999 g/mol)

The properties of the diatomic ideal gas were taken from the JANAF Thermochemical Tables[a]. The volumetric properties of the real gas were not needed and were not evaluated.

1.5.5.47. Si, silicon (formula weight = 28.086 g/mol)

The properties of silicon were taken from the compilation of Hultgren and others (1973). The volumetric properties were not needed and, therefore, were not evaluated.

1.5.5.48. SiO_2 (formula weight = 60.084 g/mol)

The data evaluated in this study required a knowledge of two polymorphs of SiO_2: quartz and cristobalite.

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[a]JANAF Thermochemical Tables, looseleaf pages for 1977 issued by Dow Chemical Company, 1707 Building, Midland, Michigan.

Table 283. Sources of thermophysical data for antigorite, $Mg_{48}Si_{34}O_{85}(OH)_{62}$.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Kunze, 1961	volume	X-ray	1	298	1.01	0.001
King and others, 1967	heat capacity	low-T. cal.	10	206-296	1.01	0.002±0.073
King and others, 1967	rel. enthalpy	drop cal.	11	406-848	1.01	0.289±0.251
King and others, 1967	entropy	low-T. cal.	1	298	1.01	0.0

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 284. Sources of thermochemical data for antigorite, $Mg_{48}Si_{34}O_{85}(OH)_{62}$.

Reaction	Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°_f(298.15 K) Third Law, kJ	H°_f(298.15 K) kJ/mol
DH	Evans and others, 1976	Gas- & solid-medium pressure apparatus	5 pr	753-933	2.0-15.0	2168.159±30.183	-71409.070
DH	Hemley and others, 1977b	H_4SiO_4 concentration	1 pr	775-799	1.0	2201.949±21.067	-71375.289
	This Study						-71397.109

Reactions:

DH $Mg_{48}Si_{34}O_{85}(OH)_{62}$[antigorite] = 18 Mg_2SiO_4[forsterite] + 4 $Mg_3Si_4O_{10}(OH)_2$[talc] + 27 H_2O[g]

1.5.5.48.1. Quartz

The thermodynamic properties of quartz were taken from the compilation of Robie and others (1978) after adjustment to 1.01 bars. The sources for the volumetric data are given in table 285. In addition, the volumetric data were constrained to conform to the alpha-beta transition for quartz. Table 286 contains the sources for the experimental data on the transition. The data are in good agreement.

1.5.5.48.2. Cristobalite

The thermodynamic data for cristobalite were taken from the JANAF Thermochemical Tables (Stull and Prophet, 1971). The volumetric data are cited by source on table 287.

1.5.5.49. Constants

Tables 288 and 289 contain the constants for the energy- and volume-related functions as given in section 1.5.3. The range is given in parentheses after the formula and name (if applicable). The precision of the functions is given on Tables 12 through 145.

Table 285. Sources of volumetric data for quartz, SiO_2.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Adams and others, 1919	(V-V°)/V°	dilatometry	18	298	2000-12000	0.05±0.17
Olinger and Halleck, 1976	V/V°	dilatometry	15	293	33000-120000	3.19±2.25
Vaidya and others, 1973	V/V°	dilatometry	9	298	5000-45000	-0.25±0.22
Jay, 1933	volume	dilatometry	9	291-1003	1.01	0.11±0.17

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 286. Sources of data on the alpha - beta transition in quartz, SiO_2.

Source	Method	No. of Points	Range Temperature (K)	Range Pressure (kb)	H°(298.15 K) Third Law, kJ
Koster van Groos and ter Heege, 1973	e.m.f.	48	845-1033	0.001-10.0	-0.577±0.003
Yoder, 1950	Solid-medium pressure apparatus	11	845-1088	0.001-10.0	-0.574±0.003
Cohen and Klement, 1967	Solid-medium pressure apparatus	48	961-1641	4.4-35.1	-0.578±0.027
This Study					-0.577

Table 287. Sources of thermophysical data for cristobalite, SiO_2.

Source	Data type	Method	Number of points	Range		Percent error[a]
				Temperature (K)	Pressure (bars)	
Johnson and Andrews, 1956	volume(alpha)		5	296-481	1.01	0.0±0.10
Johnson and Andrews, 1956	volume(beta)		8	492-1411	1.01	0.0±0.11

[a]The tabulated numbers represent the unweighted, average standard error of estimate for data in the set from the calculated value and the 1-sigma deviation of the errors about the average. Refer to text for details.

Table 288. Constants for energy-related functions in section 1.5.3.

Formula, (temperature range in kelvins)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
Al (c), (200-933.25)	-2.05250×10^{5}	-2.54841×10^{2}	0.0	-1.28573×10^{2}	2.76424×10^{1}	-4.07067×10^{-3}	1.57641×10^{-5}
Al (l), (933.25-1800)	0.0	7.64359×10^{3}	0.0	-1.45759×10^{2}	3.1 7.65×10^{1}	0.0	0.0
AlOOH Boehmite, (200-1250)	5.82075×10^{5}	-8.77120×10^{5}	-2.28992×10^{3}	-1.28729×10^{3}	1.87814×10^{2}	6.17670×10^{-3}	0.0
AlOOH Diaspore, (200-1250)	2.92012×10^{5}	-8.93662×10^{5}	-1.81222×10^{3}	-1.06013×10^{3}	1.55894×10^{2}	-1.69804×10^{-3}	0.0
$Al(OH)_3$ Gibbsite, (200-1250)	7.91422×10^{5}	-1.10591×10^{6}	-2.90212×10^{3}	-1.62610×10^{3}	2.36699×10^{2}	2.38585×10^{-2}	0.0
Al_2O_3 Corundum, (200-1800)	4.72841×10^{4}	-1.54782×10^{6}	-2.56161×10^{3}	-1.59146×10^{3}	2.38320×10^{2}	-2.06378×10^{-2}	9.41963×10^{-6}
Al_2SiO_5 Andalusite, (200-1800)	1.66755×10^{6}	-2.34464×10^{6}	-6.11720×10^{3}	-3.46104×10^{3}	5.10336×10^{2}	-9.59010×10^{-2}	6.45249×10^{-5}
Al_2SiO_5 Kyanite, (200-1800)	1.91390×10^{6}	-2.33903×10^{6}	-6.56191×10^{3}	-3.65555×10^{3}	5.34515×10^{2}	-1.00205×10^{-1}	6.69583×10^{-5}
Al_2SiO_5 Sillimanite, (200-1800)	2.73570×10^{6}	-2.31359×10^{6}	-7.42977×10^{3}	-4.05054×10^{3}	5.92346×10^{2}	-1.31153×10^{-1}	9.43392×10^{-5}
$Al_2Si_2O_5(OH)_4$ Kaolinite, (200-1250)	2.13572×10^{6}	-3.64741×10^{6}	-9.33595×10^{3}	-5.46910×10^{3}	8.17824×10^{2}	-9.20418×10^{-2}	0.0
$Al_2Si_2O_5(OH)_4$ Dickite, (200-1250)	1.80999×10^{6}	-3.66515×10^{6}	-7.92102×10^{3}	-4.65599×10^{3}	6.95678×10^{2}	-3.00884×10^{-2}	0.0
$Al_2Si_2O_5(OH)_4$ Halloysite, (200-1250)	5.20215×10^{5}	-3.68344×10^{6}	-6.38570×10^{3}	-4.05280×10^{3}	6.19577×10^{2}	-1.79153×10^{-2}	0.0
$Al_2Si_4O_{10}(OH)_2$ Pyrophyllite, (200-1250)	4.01105×10^{6}	-5.04493×10^{6}	-1.30750×10^{4}	-7.39476×10^{3}	1.09440×10^{3}	-1.64948×10^{-1}	1.14631×10^{-4}
C Graphite, (200-1800)	7.48070×10^{5}	2.15300×10^{4}	-1.03230×10^{3}	-4.66151×10^{2}	6.31600×10^{1}	-5.73400×10^{-3}	1.80790×10^{-6}
CO (g), (200-1800)	1.14564×10^{5}	-8.57737×10^{4}	0.0	5.31939×10^{1}	2.49304×10^{1}	5.11676×10^{-3}	-2.25949×10^{-6}

Table 288. Continued

Formula, (temperature range in kelvins)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
CO_2 (g), (200-1800)	5.72343×10^{5}	-3.22626×10^{5}	-8.92065×10^{2}	-3.55944×10^{2}	8.24113×10^{1}	0.0	-5.46484×10^{-7}
Ca (c), (200-720)	-2.20152×10^{5}	-1.86563×10^{4}	3.64127×10^{2}	7.62562×10^{1}	0.0	9.83620×10^{-3}	9.72458×10^{-6}
Ca (c), (720-1112)	0.0	1.49497×10^{4}	-7.53816	3.71052×10^{1}	0.0	2.05709×10^{-2}	0.0
Ca (l), (1112-1755)	0.0	1.58488×10^{4}	0.0	-1.14367×10^{2}	2.92754×10^{1}	0.0	0.0
Ca (g), (1755-1800)	0.0	1.84078×10^{5}	-8.35017	3.19488×10^{1}	2.14177×10^{1}	-3.02477×10^{-4}	2.25282×10^{-7}
$CaAl_2SiO_6$ Ca-Al Clinopyroxene, (200-1800)	-2.76402×10^{6}	-3.11084×10^{6}	-2.16570×10^{3}	-1.95915×10^{3}	3.22156×10^{2}	0.0	0.0
$CaAl_2Si_2O_8$ Anorthite, (200-1800)	3.14402×10^{6}	-3.83663×10^{6}	-9.38321×10^{3}	-5.32656×10^{3}	7.96492×10^{2}	-1.44198×10^{-1}	1.02906×10^{-4}
$CaAl_4Si_2O_{10}(OH)_2$ Margarite, (200-1250)	0.0	-5.74866×10^{6}	-7.50967×10^{3}	-4.97842×10^{3}	7.68405×10^{2}	-9.70931×10^{-3}	0.0
$CaCO_3$ Calcite, (200-1800)	0.0	-1.10747×10^{6}	-1.11449×10^{3}	-8.37835×10^{2}	1.39006×10^{2}	1.43039×10^{-2}	0.0
$CaCO_3$ Aragonite, (200-1800)	0.0	-1.10921×10^{6}	-1.04452×10^{3}	-8.11951×10^{2}	1.35497×10^{2}	1.15890×10^{-2}	0.0
CaO Lime, (200-1800)	-2.55577×10^{5}	-5.99178×10^{5}	-4.31990×10^{2}	-4.20068×10^{2}	7.16851×10^{1}	-3.08248×10^{-3}	2.23862×10^{-6}
$CaSiO_3$ Wollastonite, (200-1398.15)	0.0	-1.52204×10^{6}	-1.68000×10^{3}	-1.17043×10^{3}	1.85955×10^{2}	-3.60167×10^{-3}	-6.39008×10^{-7}
$CaSiO_3$ Cyclowollastonite, (200-1800)	-5.46489×10^{5}	-1.52204×10^{6}	-9.42731×10^{2}	-8.77640×10^{2}	1.49650×10^{2}	0.0	0.0
$CaAl_2Si_2O_6(OH)_2$ Bicchulite, (200-1250)	0.0	-3.99020×10^{6}	-5.20338×10^{3}	-3.52194×10^{3}	5.51767×10^{2}	-1.21058×10^{-2}	0.0
$CaAl_2Si_2O_7$ Gehlenite, (200-1800)	1.49598×10^{6}	-3.67055×10^{6}	-6.24654×10^{3}	-3.80818×10^{3}	5.86351×10^{2}	-6.60911×10^{-2}	3.80365×10^{-5}

Table 288. Continued

Formula, (temperature range in kelvins)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
$Ca_2Al_2Si_3O_{10}(OH)_2$ Prehnite, (200-1250)	2.05022×10^{6}	-5.65525×10^{6}	-9.60611×10^{3}	-5.84599×10^{3}	8.88366×10^{2}	-4.01441×10^{-2}	0.0
$Ca_2Al_3Si_3O_{12}(OH)$ Zoisite, (200-1250)	2.04129×10^{6}	-6.32506×10^{6}	-1.04175×10^{4}	-6.32203×10^{3}	9.56365×10^{2}	-4.39555×10^{-2}	0.0
Ca_2SiO_4 Alpha, (1710-1800)	0.0	-2.22496×10^{6}	0.0	-1.05191×10^{3}	1.99600×10^{2}	0.0	0.0
Ca_2SiO_4 Bredigite, (200-1710)	0.0	-2.20583×10^{6}	0.0	-8.04599×10^{2}	1.61526×10^{2}	0.0	1.89495×10^{-5}
Ca_2SiO_4 Ca Olivine, (200-1200)	-2.36007×10^{6}	-2.23871×10^{6}	1.65638×10^{3}	2.39144×10^{2}	0.0	1.06586×10^{-1}	-8.15012×10^{-5}
Ca_2SiO_4 Larnite, (200-970)	0.0	-2.15665×10^{6}	-2.09476×10^{3}	-1.53830×10^{3}	2.49720×10^{2}	0.0	0.0
$Ca_3Al_2Si_3O_{12}$ Grossularite, (200-1800)	1.76828×10^{6}	-6.11005×10^{6}	-1.07953×10^{4}	-6.59048×10^{3}	9.94708×10^{2}	-1.06084×10^{-1}	4.94577×10^{-5}
Ca_3SiO_5 Hatrurite, (200-1800)	0.0	-2.74033×10^{6}	-2.84600×10^{3}	-2.08607×10^{3}	3.38162×10^{2}	-2.81920×10^{-3}	0.0
$Ca_3Si_2O_7$ Rankinite, (200-1650)	2.11044×10^{5}	-3.70604×10^{6}	-4.07831×10^{3}	-2.85586×10^{3}	4.57070×10^{2}	-1.50836×10^{-2}	0.0
$Ca_4Al_6Si_6O_{24}(CO_3)$ Meionite, (200-1800)	-9.14788×10^{6}	-1.30405×10^{7}	-9.97380×10^{3}	-8.49709×10^{3}	1.40091×10^{3}	0.0	0.0
Fe (c), (alpha), (200-1042)[a]	4.67900×10^{6}	1.29860×10^{5}	-6.43980×10^{3}	-3.09983×10^{3}	4.40747×10^{2}	-1.87588×10^{-1}	1.83975×10^{-4}
Fe (c), (alpha'), (1042-1800)[a]	3.11294×10^{8}	1.72901×10^{6}	-3.78574×10^{4}	-9.46728×10^{3}	1.07515×10^{3}	-6.56081×10^{-2}	0.0
Fe (c), (gamma), (1184-1665)	0.0	8.45146×10^{3}	0.0	-1.03591×10^{2}	2.39743×10^{1}	4.18400×10^{-3}	0.0
$Fe_{.947}O$ Wustite, (200-1800)	0.0	-2.35710×10^{5}	-3.66286×10^{2}	-3.95757×10^{2}	7.29225×10^{1}	-6.83700×10^{-3}	8.66116×10^{-6}
$FeSiO_3$ Ferrosilite, (200-1800)	-2.87221×10^{6}	-1.13188×10^{6}	0.0	-5.40441×10^{2}	1.07120×10^{2}	1.72796×10^{-2}	-8.84986×10^{-6}

[a] The functions in section 1.5.3, using the fitted coefficients for iron in table 288, do not accurately describe the thermodynamic properties for iron over a temperature interval approximately 30°C below to 10°C above the alpha - alpha' lambda transition at 1042 K.

Table 288. Continued

Formula, (temperature range in kelvins)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
Fe_2O_3 Hematite (alpha), (200-955.5)[b]	2.12782×10^{6}	-6.32880×10^{5}	-6.85832×10^{3}	-3.92482×10^{3}	5.88529×10^{2}	-2.26663×10^{-1}	2.66461×10^{-4}
Fe_2O_3 Hematite (alpha'), (955.5-1800)[b]	4.82281×10^{8}	2.19790×10^{6}	-6.74698×10^{4}	-1.77835×10^{4}	2.06675×10^{3}	-1.32541×10^{-1}	0.0
Fe_2SiO_4 Fayalite, (200-1800)	1.98186×10^{6}	-1.26795×10^{6}	-5.91318×10^{3}	-3.39012×10^{3}	5.15172×10^{2}	-1.20206×10^{-1}	9.73963×10^{-5}
Fe_3O_4 Magnetite (alpha), (200-848.5)[c]	4.99456×10^{6}	-7.77610×10^{5}	-1.40898×10^{4}	-7.94562×10^{3}	1.19482×10^{3}	-5.96710×10^{-1}	8.08724×10^{-4}
Fe_3O_4 Magnetite (alpha'), (848.5-1800)[c]	1.13548×10^{9}	8.60687×10^{6}	-2.71125×10^{5}	-8.39335×10^{4}	1.02102×10^{4}	-1.50333	4.45065×10^{-4}
H_2 (g), (200-1800)	-5.10406×10^{5}	2.03250×10^{4}	4.10165×10^{2}	1.29375×10^{2}	7.44240	5.85357×10^{-3}	-1.38995×10^{-6}
H_2O (water), (273.15-373.15)	1.10338×10^{6}	-2.28245×10^{5}	0.0	-1.84121×10^{2}	4.20228×10^{1}	3.49132×10^{-2}	0.0
H_2O (g), (200-1800)	-1.31077×10^{5}	-1.87339×10^{5}	2.99188×10^{2}	1.55636×10^{2}	1.04381×10^{1}	1.29775×10^{-2}	-4.46885×10^{-6}
Mg (c), (200-922)	1.09922×10^{5}	9.43865×10^{3}	-4.20253×10^{2}	-3.18568×10^{2}	5.45289×10^{1}	-1.41605×10^{-2}	2.16245×10^{-5}
Mg (l), (922-1378)	0.0	1.16498×10^{4}	0.0	-8.67553×10^{1}	2.20919×10^{1}	5.43908×10^{-3}	0.0
Mg (g), (200-1800)	0.0	1.51165×10^{5}	0.0	3.01177×10^{1}	2.07861×10^{1}	0.0	0.0
$MgCO_3$ Magnesite, (200-1800)	4.98826×10^{5}	-9.94803×10^{5}	-2.00686×10^{3}	-1.22914×10^{3}	1.86847×10^{2}	0.0	0.0
MgO Periclase, (200-1800)	-3.73496×10^{5}	-5.06544×10^{5}	-4.78258×10^{2}	-4.32701×10^{2}	7.08871×10^{1}	-3.05096×10^{-3}	1.97050×10^{-6}
$Mg(OH)_2$ Brucite, (200-1250)	0.0	-8.08692×10^{5}	-1.75140×10^{3}	-1.16892×10^{3}	1.80978×10^{2}	-3.19863×10^{-3}	0.0
$MgSiO_3$ Clinoenstatite, (200-968.5)	-4.33797×10^{5}	-1.44239×10^{6}	-1.31078×10^{3}	-1.01158×10^{3}	1.62362×10^{2}	0.0	0.0

[b]The functions in section 1.5.3, using the fitted coefficients for hematite in table 288, do not accurately describe the thermodynamic properties for hematite over a temperature interval approximately 30°C below to 10°C above the alpha - alpha' lambda transition at 955.50 K.

[c]The function in section 1.5.3, using the fitted coefficients for magnetite in table 288, do not accurately describe the thermodynamic properties of magnetite over a temperature interval approximately 30°C below to 10°C above the alpha - alpha' lambda transition at 848.50 K.

Table 288. Continued

Formula, (temperature range in kelvins)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
$MgSiO_3$ Enstatite, (200-1257.4)	1.87801×10^{5}	-1.42478×10^{6}	-2.12685×10^{3}	-1.35648×10^{3}	2.07387×10^{2}	-6.91249×10^{-3}	0.0
$MgSiO_3$ Protoenstatite, (1257.4-1800)	0.0	-1.42543×10^{6}	-1.34677×10^{3}	-9.74472×10^{2}	1.57987×10^{2}	0.0	0.0
Mg_2SiO_4 Forsterite, (200-1800)	-5.96175×10^{5}	-2.03090×10^{6}	-1.95051×10^{3}	-1.48847×10^{3}	2.37767×10^{2}	0.0	0.0
$Mg_3Si_2O_5(OH)_4$ Chrysotile, (200-1250)	1.05526×10^{6}	-3.91400×10^{6}	-7.44838×10^{3}	-4.63858×10^{3}	7.04568×10^{2}	-1.88092×10^{-2}	0.0
$Mg_3Si_4O_{10}(OH)_2$ Talc, (200-1250)	0.0	-5.39026×10^{6}	-8.41302×10^{3}	-5.39579×10^{3}	8.24301×10^{2}	-2.41645×10^{-2}	0.0
$Mg_7Si_8O_{22}(OH)_2$ Anthophyllite, (200-1250)	5.53225×10^{6}	-1.09427×10^{7}	-2.37023×10^{4}	-1.40164×10^{4}	2.10106×10^{3}	-2.29152×10^{-1}	1.08662×10^{-4}
$Mg_{48}Si_{34}O_{85}(OH)_{62}$ Antigorite, (200-1250)	1.69609×10^{7}	-6.41927×10^{7}	-1.20609×10^{5}	-7.51253×10^{4}	1.14157×10^{4}	-3.10333×10^{-1}	0.0
O_2 (g), (200-1800)	1.84663×10^{5}	5.68075×10^{4}	-1.70675×10^{2}	-1.75052×10^{1}	3.54525×10^{1}	3.17977×10^{-3}	-1.85549×10^{-6}
Si (c), (200-1665)	-1.48020×10^{5}	1.75295×10^{3}	-1.77189×10^{2}	-1.83356×10^{2}	3.17050×10^{1}	2.81373×10^{-4}	0.0
Si (l), (1665-1800)	0.0	4.84612×10^{4}	0.0	-9.78143×10^{1}	2.55224×10^{1}	0.0	0.0
SiO_2 Quartz (alpha), (200-844)	0.0	-8.42859×10^{5}	-7.78110×10^{2}	-5.29534×10^{2}	8.32575×10^{1}	1.09794×10^{-2}	0.0
SiO_2 Quartz (beta), (844-1800)	0.0	-8.62517×10^{5}	0.0	-3.00970×10^{2}	5.89128×10^{1}	5.01976×10^{-3}	0.0
SiO_2 Cristobalite (alpha), (200-523)	0.0	-8.41305×10^{5}	-6.70636×10^{2}	-4.54294×10^{2}	7.15824×10^{1}	2.53644×10^{-2}	-3.27023×10^{-5}
SiO_2 Cristobalite (beta), (523-1800)	-4.14084×10^{6}	-8.73998×10^{5}	0.0	-3.86787×10^{2}	7.27781×10^{1}	6.43199×10^{-4}	0.0

Table 289. Constants for volume-related functions in section 1.5.3. The dashes (---) indicate the parameters were not determined.

Formula, (temperature range in kelvins)	b_1	b_2	b_3	b_4	b_5
Al (c), (200-933.25)	---	---	---	---	---
Al (l), (933.25-1800)	---	---	---	---	---
AlOOH Boehmite, (200-1250)	1.86380×10^{1}	3.00666×10^{-3}	0.0	-3.00000×10^{-5}	0.0
AlOOH Diaspore, (200-1250)	1.74058×10^{1}	1.18889×10^{-3}	0.0	-3.67156×10^{-5}	0.0
$Al(OH)_3$ Gibbsite, (200-1250)	3.17958×10^{1}	5.37300×10^{-4}	0.0	-6.29400×10^{-7}	0.0
Al_2O_3 Corundum, (200-1800)	2.52017×10^{1}	6.55518×10^{-4}	0.0	-6.02751×10^{-6}	2.01149×10^{-1}
Al_2SiO_5 Andalusite, (200-1800)	5.00729×10^{1}	1.73719×10^{-3}	5.36253×10^{-1}	-2.16986×10^{-5}	7.70038×10^{-1}
Al_2SiO_5 Kyanite, (200-1800)	4.23174×10^{1}	1.24871×10^{-3}	2.29753×10^{-1}	8.04308×10^{-6}	1.43243
Al_2SiO_5 Sillimanite, (200-1800)	4.91338×10^{1}	9.35712×10^{-4}	4.23863×10^{-1}	-2.61363×10^{-5}	4.48630×10^{-1}
$Al_2Si_2O_5(OH)_4$ Kaolinite, (200-1250)	9.84196×10^{1}	3.56979×10^{-3}	0.0	-4.04420×10^{-4}	0.0
$Al_2Si_2O_5(OH)_4$ Dickite, (200-1250)	9.81973×10^{1}	3.70000×10^{-3}	0.0	-4.00000×10^{-4}	0.0
$Al_2Si_2O_5(OH)_4$ Halloysite, (200-1250)	9.82973×10^{1}	3.70000×10^{-3}	0.0	-4.00000×10^{-4}	0.0
$Al_2Si_4O_{10}(OH)_2$ Pyrophyllite, (200-1250)	1.26819×10^{2}	1.73097×10^{-3}	8.15952×10^{-1}	-7.24744×10^{-6}	0.0
C Graphite, (200-1800)	---	---	---	---	---
CO (g), (200-1800)	---	---	---	---	---

Table 289. Continued

Formula, (temperature range in kelvins)	b_1	b_2	b_3	b_4	b_5
CO_2 (g), (200-1800)	---	---	---	---	---
Ca (c), (200-720)	---	---	---	---	---
Ca (c), (720-1112)	---	---	---	---	---
Ca (l), (1112-1755)	---	---	---	---	---
Ca (g), (1755-1800)	---	---	---	---	---
$CaAl_2SiO_6$ Ca-Al Clinopyroxene, (200-1800)	6.28408×10^{1}	1.89768×10^{-3}	4.60438×10^{-1}	-4.88417×10^{-5}	0.0
$CaAl_2Si_2O_8$ Anorthite, (200-1800)	9.95773×10^{1}	1.28176×10^{-3}	0.0	-1.10185×10^{-4}	7.67851×10^{-1}
$CaAl_4Si_2O_{10}(OH)_2$ Margarite, (200-1250)	1.32864×10^{2}	3.04606×10^{-3}	0.0	-3.67641×10^{-4}	0.0
$CaCO_3$ Calcite, (200-1800)	3.60246×10^{1}	2.52024×10^{-4}	8.69853×10^{-2}	-3.63779×10^{-5}	6.45538×10^{-1}
$CaCO_3$ Aragonite, (200-1800)	4.28575×10^{1}	3.63164×10^{-5}	1.85897×10^{-2}	-2.48053×10^{-4}	-8.73263
CaO Lime, (200-1800)	1.57869×10^{1}	7.79428×10^{-4}	2.46416×10^{-1}	0.0	6.50708×10^{-1}
$CaSiO_3$ Wollastonite, (200-1398.15)	3.88495×10^{1}	4.62101×10^{-4}	-1.30789	-1.82503×10^{-5}	1.29086
$CaSiO_3$ Cyclowollastonite, (200-1800)	3.65365×10^{1}	8.26635×10^{-4}	4.23913×10^{-1}	1.01459×10^{-5}	3.21801
$CaAl_2Si_2O_6(OH)_2$ Bicchulite, (200-1250)	1.02427×10^{2}	3.75930×10^{-3}	0.0	-1.32974×10^{-4}	0.0
$CaAl_2Si_2O_7$ Gehlenite, (200-1800)	8.95072×10^{1}	2.48640×10^{-3}	0.0	-4.09381×10^{-5}	0.0

Table 289. Continued

Formula, (temperature range in kelvins)	b_1	b_2	b_3	b_4	b_5
$Ca_2Al_2Si_3O_{10}(OH)_2$ Prehnite, (200-1250)	1.38906×10^{2}	5.12338×10^{-3}	0.0	-2.23955×10^{-4}	0.0
$Ca_2Al_3Si_3O_{12}(OH)$ Zoisite, (200-1250)	1.35236×10^{2}	4.97840×10^{-3}	0.0	-1.65560×10^{-4}	0.0
Ca_2SiO_4 Alpha, (1710-1800)	5.17315×10^{1}	1.90000×10^{-3}	0.0	-3.28000×10^{-5}	0.0
Ca_2SiO_4 Bredigite, (200-1710)	5.14335×10^{1}	1.90000×10^{-3}	0.0	-3.30000×10^{-5}	0.0
Ca_2SiO_4 Ca Olivine, (200-1200)	5.85137×10^{1}	2.00000×10^{-3}	0.0	-3.50000×10^{-5}	0.0
Ca_2SiO_4 Larnite, (200-970)	5.12763×10^{1}	8.21518×10^{-4}	2.12884×10^{-1}	-3.24000×10^{-5}	0.0
$Ca_3Al_2Si_3O_{12}$ Grossularite, (200-1800)	1.23151×10^{2}	3.35891×10^{-3}	5.69824×10^{-1}	-6.43965×10^{-5}	8.29661×10^{-1}
Ca_3SiO_5 Hatrurite, (200-1800)	7.22620×10^{1}	1.04235×10^{-3}	4.57211×10^{-1}	-4.00000×10^{-5}	0.0
$Ca_3Si_2O_7$ Rankinite, (200-1650)	9.60060×10^{1}	1.35971×10^{-3}	2.47665×10^{-1}	-8.00000×10^{-5}	0.0
$Ca_4Al_6Si_6O_{24}(CO_3)$ Meionite, (200-1800)	3.35917×10^{2}	5.63126×10^{-3}	0.0	-4.36470×10^{-4}	0.0
Fe (c), (alpha), (200-1042)[a]	7.01063	2.79272×10^{-4}	0.0	-4.08527×10^{-6}	0.0
Fe (c), (alpha'), (1042-1800)[a]	7.09200	0.0	0.0	0.0	0.0
Fe (c), (gamma), (1184-1665)	7.09200	0.0	0.0	0.0	0.0
$Fe_{.947}O$ Wustite, (200-1800)	1.19646×10^{1}	0.0	0.0	-6.20724×10^{-6}	7.49475×10^{-2}
$FeSiO_3$ Ferrosilite, (200-1800)	3.26273×10^{1}	1.21117×10^{-3}	0.0	-7.11674×10^{-5}	0.0

[a]The functions in section 1.5.3, using the fitted coefficients for iron in table 289, do not accurately describe the thermophysical properties for iron over a temperature interval approximately 30°C below to 10°C above the alpha - alpha' lambda transition at 1042 K.

Table 289. Continued

Formula, (temperature range in kelvins)	b_1	b_2	b_3	b_4	b_5
Fe_2O_3 Hematite (alpha), (200-955.5)[b]	$2.96670x10^{1}$	$1.17167x10^{-3}$	0.0	$-1.01344x10^{-5}$	$2.58748x10^{-1}$
Fe_2O_3 Hematite (alpha'), (955.5-1800)[b]	$2.96670x10^{1}$	$1.17167x10^{-3}$	0.0	$-1.01344x10^{-5}$	$2.58748x10^{-1}$
Fe_2SiO_4 Fayalite, (200-1800)	$4.57046x10^{1}$	$1.48633x10^{-3}$	0.0	$-3.48762x10^{-5}$	0.0
Fe_3O_4 Magnetite (alpha), (200-848.5)[c]	$4.43930x10^{1}$	$4.38323x10^{-4}$	0.0	$-2.58503x10^{-5}$	0.0
Fe_3O_4 Magnetite (alpha'), (848.5-1800)[c]	$4.45420x10^{1}$	0.0	0.0	0.0	0.0
H_2 (g), (200-1800)	---	---	---	---	---
H_2O (water), (273.15-373.15)	---	---	---	---	---
H_2O (g), (200-1800)	---	---	---	---	---
Mg (c), (200-922)	---	---	---	---	---
Mg (l), (922-1378)	---	---	---	---	---
Mg (g), (200-1800)	---	---	---	---	---
$MgCO_3$ Magnesite, (200-1800)	$2.78494x10^{1}$	$5.65880x10^{-4}$	0.0	$-3.60075x10^{-5}$	0.0
MgO Periclase, (200-1800)	$1.11195x10^{1}$	$4.17881x10^{-4}$	0.0	$-6.09873x10^{-6}$	0.0
$Mg(OH)_2$ Brucite, (200-1250)	$2.42379x10^{1}$	$5.3394/x10^{-4}$	0.0	0.0	$2.33794x10^{-1}$
$MgSiO_3$ Clinoenstatite, (200-968.5)	$3.09763x10^{1}$	$9.97411x10^{-4}$	0.0	$-2.73873x10^{-5}$	0.0

[b]The functions in section 1.5.3, using the fitted coefficients for hematite in table 289, do not accurately describe the thermophysical properties for hematite over a temperature interval approximately 30°C below to 10°C above the alpha - alpha' lambda transition at 955.50 K.

[c]The functions in section 1.5.3, using the fitted coefficients for magnetite in table 289, do not accurately describe the thermophysical properties of magnetite over a temperature interval approximatley 30°C below to 10°C above the alpha - alpha' lambda transition at 848.50 K.

Table 289. Continued

Formula, (temperature range in kelvins)	b_1	b_2	b_3	b_4	b_5
$MgSiO_3$ Enstatite, (200-1257.4)	3.05149×10^{1}	1.04744×10^{-3}	3.47023×10^{-1}	-1.73729×10^{-5}	3.94505×10^{-1}
$MgSiO_3$ Protoenstatite, (1257.4-1800)	3.20608×10^{1}	9.29762×10^{-4}	0.0	-2.58376×10^{-5}	0.0
Mg_2SiO_4 Forsterite, (200-1800)	4.22835×10^{1}	1.96402×10^{-3}	6.52600×10^{-1}	-2.22563×10^{-5}	5.42082×10^{-1}
$Mg_3Si_2O_5(OH)_4$ Chrysotile, (200-1250)	9.80393×10^{1}	2.08435×10^{-3}	0.0	0.0	8.61502
$Mg_3Si_4O_{10}(OH)_2$ Talc, (200-1250)	1.24360×10^{2}	2.92124×10^{-3}	0.0	0.0	1.07237×10^{1}
$Mg_7Si_8O_{22}(OH)_2$ Anthophyllite, (200-1250)	2.63636×10^{2}	7.62631×10^{-4}	0.0	-3.40187×10^{-5}	0.0
$Mg_{48}Si_{34}O_{85}(OH)_{62}$ Antigorite, (200-1250)	1.60250×10^{3}	3.59060×10^{-2}	0.0	0.0	1.35952×10^{2}
O_2 (g), (200-1800)	---	---	---	---	---
Si (c), (200-1685)	---	---	---	---	---
Si (l), (1685-1800)	---	---	---	---	---
SiO_2 Quartz (alpha), (200-844)	2.21819×10^{1}	1.35725×10^{-3}	0.0	-4.27012×10^{-5}	0.0
SiO_2 Quartz (beta), (844-1800)	2.35794×10^{1}	0.0	0.0	-4.73106×10^{-5}	0.0
SiO_2 Cristobalite (alpha), (200-523)	2.50374×10^{1}	2.57716×10^{-3}	0.0	-6.46000×10^{-5}	0.0
SiO_2 Cristobalite (beta), (523-1800)	2.72307×10^{1}	2.11894×10^{-4}	0.0	-6.46000×10^{-5}	0.0

1.6. Symbols and Units

The following symbols were used in the text, tables, and data summaries.

Symbol	Units	Meaning
$a_{1,i}$; $a_{2,i}$; $a_{3,i}$; $a_{4,i}$; $a_{5,i}$; $a_{6,i}$; $a_{7,i}$	--	Fitted coefficients describing the thermodynamic properties of phase i as a function of temperature according to equations 22 through 27 in text.
a_{1,P_r}; a_{2,P_r}	--	Fitted coefficient describing the thermodynamic properties of silicic acid in aqueous fluids as a function of temperature at a reference pressure according to equation 28 in text.
$b_{1,i}$; $b_{2,i}$; $b_{3,i}$; $b_{4,i}$; $b_{5,1}$	--	Fitted coefficients describing the volume and thermodynamic properties of phase i as a function of temperature and pressure according to equations 23 through 27 in text.
$^\circ$	--	Superscript designating the standard state of a phase
α_p	K^{-1}	Isobaric coefficient of thermal expansion. Designation of $(\partial V/\partial T)_p/V)$
β_T	bar^{-1}	Isothermal coefficient of compressibility. Designation of $-(\partial V/\partial P)_T/V)$
C_i	J/(g•K)	Specific heat of rock oxide component i
C_p; $C_{p,i}$	J/(mol•K)	Isobaric molar heat capacity at 1 atmosphere pressure. Subscript i identifies the i th phase.
C_p°	J/(mol•K)	Standard isobaric molar heat capacity at 1 atmosphere pressure.
$C_{p,i}^{'}$	J/(mol•K)	Isobaric molar heat capacity of mineral fictive structural component i.

Symbol	Units	Meaning
E	volts	Standard electrochemical potential in volts
G; $G_{T,P}$	J/mol	Molar Gibbs energy. The subscripts T and P designate the temperature and pressure conditions, respectively, associated with the Gibbs energy property.
G_i	J/mol	Molar Gibbs energy of the i th phase.
$[G^\circ_T - H^\circ_{298}]/T$	J/(mol·K)	Standard molar Gibbs energy function
$\Delta G^\circ_{f,e}$	J/mol	Standard molar Gibbs energy of formation from the elements
$\Delta G^\circ_{f,ox}$	J/mol	Standard molar Gibbs energy of formation from the oxides
$\Delta G_{r_{T,P}}$; $\Delta G_{r_{T,P_r}}$	J/mol	Gibbs energy of reaction. The subscripts T, P, and P_r designate the temperature and pressure or reference pressure conditions, respectively, of the Gibbs energy of reaction property.
H; H_T; $H_{T,P}$	J/mol	Molar enthalpy. The subscripts T and P designate the temperature and pressure conditions, respectively, of the enthalpy property.
H_0	J/mol	Zero point molar enthalpy. Enthalpy at 0 K and 101.325 kPa.
$H^\circ_T - H^\circ_{298}$	J/mol	Relative standard molar enthalpy. Base is H° at 298.15 K and 101.325 kPa
$H_T - H_{T_r}$	J/mol	Relative molar enthalpy. The subscripts T and T_r designate the temperature and reference temperature associated with the relative enthalpy property.
$H^\circ_{T,i} - H^\circ_{T_r,i}$	J/mol	Relative standard molar enthalpy of fictive structural component i. The subscripts T and T_r designate the temperature and reference temperature associated with the relative enthalpy property.

Symbol	Units	Meaning
$\Delta H^{\circ}_{f,e}$	J/mol	Standard molar enthalpy of formation from the elements
$\Delta H^{\circ}_{f,ox}$	J/mol	Standard molar enthalpy of formation from the oxides
ΔH_r	J	Enthalpy of reaction
i	--	Index designating a mineral or fictive structural component species
j	--	Index designating the number of phases in a reaction
ln K	--	Natural log of the equilibrium constant for a reaction.
log $K^{\circ}_{f,e}$	--	$\log_{10}$ of the standard equilibrium constant for formation from the elements
log $K^{\circ}_{f,ox}$	--	$\log_{10}$ of the standard equilibrium constant for formation from the oxides
M	mol	Designation of (grams of sample/ molar weight of sample).
n	--	Number of electrons transferred during an electrochemical reaction.
N_i	mol	Stoichiometric coefficient for phase i in a reaction. Value is positive for reaction products and negative for reactants.
P	Pa	Absolute pressure in pascals
P_r	Pa	Reference pressure
r	--	Subscript index designating a reference state or reference material.
s	--	Subscript index designating sample material in a Differential Scanning Calorimeter measurement.

Symbol	Units	Meaning
S; S_T; $S_{T,P}$; S_{T,P_r}	J/(mol •K)	Molar entropy. Subscripts T, P, and P_r designate the temperature, pressure, or reference pressure, respectively, of the entropy property.
$S°$	J/(mol •K)	Standard molar entropy
$S_i^\dagger$	J/(mol •K)	Standard molar entropy of fictive mineral structural component i
S_0	J/(mol •K)	Zero point entropy.
$S_T - S_0$	J/(mol •K)	Calorimetric entropy.
t	sec	Time in seconds.
T	K	Absolute temperature in kelvins
T_r	K	Reference temperature, absolute scale in kelvins
V, V_T	cm^3/mol	Molar volume. The subscript T designates the temperature condition associated with the volume property.
$V°$, $V_i°$	cm^3/mol	Standard molar volume. Subscript i identifies the i th phase.
X_i	--	Mass fraction of oxide component i used to calculate the specific heat of rocks according to equation 150 in text. Designation of (grams of component i/grams of rock).

Fundamental constants used in this evaluation are given in section 1.7.

Where possible, the data have been corrected to the International Practical Temperature Scale of 1968 (Comite International des Poids et Measures, 1969). For most phase equilibria, however, this was not possible because the necessary temperature calibration data were not supplied by the authors.

The "formula weights" have been calculated to be consistent with the 1975 relative atomic masses for the elements (Commission on Atomic Weights, 1976).

1.7. Fundamental Constants, Defined Constants, and Conversion Factors from Non-SI Units to SI Units

Name	Symbol	Value and units
Fundamental constants		
Avagadro constant	N	6.022094×10^{23} mol^{-1}
Faraday constant	$\mathcal{F}$	96,487.0 J/(volts·mol)
Gas constant	R	8.3143 J/(mol·K)
Absolute temperature of the "ice point," 0°C		273.15 K
Defined units		
Standard atmosphere	atm	101.325 kPa
Standard bar	b	100.000 kPa
Thermochemical calorie	cal	4.1840 J

Conversion factors from non-SI units to SI units

0°C	=	273.15 K
1 Å	=	10^{-10} m
1 bar	=	10^5 Pa
1 atm	=	101325 Pa
1 cal	=	4.184 J
1 g cm^{-3}	=	1×10^3 Kg m^{-3}