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Recommended Standard Electrochemical Potentials and Fugacities of Oxygen for the Solid Buffers and Thermodynamic Data in the Systems Iron-Silicon-Oxygen, Nickel-Oxygen, and Copper-Oxygen

by

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with comments and additions by

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Introduction

John L. Haas, Jr. developed computer software for the simultaneously multiple regression of thermochemical data (Haas and Fisher, 1976) and examined the chemical systems iron-silicon-oxygen, nickel-oxygen, and copper-oxygen as an example of the use and application of the software. The majority of this report represents his effort on those systems through early 1989. He worked on this study in collaboration with the CODATA (Committee on Data for Science and Technology of the International Council of Scientific Unions) Task Group on Chemical Thermodynamic Tables (TGCTT) for which most of this report was prepared in January of 1988. He retired from the USGS in late 1988 and worked briefly on the project in early 1989. His intention had been to publish this study as a USGS Bulletin. However, following a review by the TGCTT in early 1989 he abandoned the effort. His study received high marks from the TGCTT and was accepted in principle with suggestions for some changes. All changes except that involving wüstite were completed. The information in this report is used by many investigator through out the world. This report provides a formal reference to that study and to follow on efforts which have been compiled for this purpose by Hemingway. The report is composed of 5 parts. The first four parts represent the original report submitted to the TGCTT, with corrections noted by Haas to members of the TGCTT in a letter dated February 27, 1988. Part five provides revised tables of thermodynamic data for most of the phases studied and they bear the number of the table that they replace (Tables 8.01 - 8.21).

the number of the table that they replace (Tables 8.01 - 8.21). These values may be compared with the original tables of thermodynamic data, figures and comparative data tables provided in Parts 1-4. Part 5 is based upon computer runs made in April of 1989 on a VAX 11/780 computer. (The use of trade, brand or product names in this report is for identification purposes only and does not constitute endorsement by the U.S. Geological Survey.) Haas has provided a copy of this version of his program to the Chemical Thermodynamics Data Center at the National Institute of Standards and Technology in Gaithersburg, Maryland, and to the USGS in the form of both fortran code for the VAX and as fortran code for IBM compatible microcomputers. An earlier version of the program is available in IBM compatible microcomputer code from the USGS as Open-File Report 88-489 A and B. Part 6 lists the current version of the software called TDM001. The original program was called PHAS20.

Recommended Standard Electrochemical Potentials and Fugacities of Oxygen for the Solid Buffers and Thermodynamic Data in the Systems Iron-Silicon-Oxygen, Nickel-Oxygen, and Copper-Oxygen

Part 1
Abstract, Table of Contents, and Text

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Recommended fugacities and standard electrochemical potentials for O_2 in the buffer pairs from 200 to 1800 K were derived from critical reviews of experimental data and thermodynamic theory. Included are C_p°, H°(T)-H°(298), [G°(T)-H°(298)]/T, S°, $\Delta_f H^\circ$, $\Delta_f G^\circ$, V°, and the coefficients of volume expansion and of volume compression for the oxide phases.

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ABSTRACT

Recommended thermodynamic data, including standard electrochemical potentials and fugacities of oxygen, are supplied for the oxygen buffers: copper-cuprite, cuprite-tenorite, nickel-bunsenite, iron-wustite, iron-magnetite, iron-quartz-fayalite, wustite-magnetite, magnetite-quartz-fayalite, and magnetite-hematite. The data for the buffers are the product of a detailed statistical evaluation of the experimental data for the copper-oxygen, nickel-oxygen, and iron-silicon-oxygen systems, using thermodynamic theory and simultaneous least-squares regression techniques.

The thermodynamic and volumetric data have been revised for each of the oxides and for fayalite. Algebraic equations are also supplied for the molar volume, heat capacity, entropy, heat content, and other thermodynamic properties of these phases.

New equations for the thermodynamic and volumetric properties of the wustite solid solution and of the metastable, stoichiometric compound, FeO, are included in the report. In evaluating the wustite solid solution, the existence of "domains" was noted but not used to derive the thermodynamic properties. In part the published data for domains are conflicting, but more often the differences in the data that indicate the existence of domains are at the level of precision for the measurements. Before serious evaluation can include this phenonemon, more precise and reproducible data are needed. The

activities of Fe, O_2, and FeO in the wustite solid solution as a function of temperature from 800 K to 1700 K are given in tables. The equations used to prepare the tables are given so that the user can calculate the properties at conditions other than those supplied. The functions describe the properties of wustite at one atmosphere from the isobaric invariant point (iron-wustite-magnetite equilibrium) to the melting curve for the solid solution. The temperature and composition of the isobaric invariant point was found to be 839.15 K and $Fe_{0.917}O$, respectively.

No attempt was made to evaluate the wustite-liquid equilibria or the properties of the liquid phase.

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CHAPTER 1

INTRODUCTION

Introduction

The experimental data from calorimetry, X-ray diffraction, and reaction equilibria for the oxides of copper, nickel, and iron, and for fayalite have been critically reviewed. The critical review identified inconsistent data. An optimization routine using thermodynamic principles gave a statistically based best fit of the valid data. The thermodynamic functions for the oxides and for fayalite and the recommended standard electrochemical potentials of nine commonly used solid oxygen buffer assemblages have been improved through this approach. In addition, the phase relations for the wustite solid solution have been found to differ considerably from the previous estimates. The thermodynamic properties of the solid solution, in particular, the partial molar properties and activities of Fe, FeO, and O_2 are in good agreement with the experimental data for wustite. However, the most important contribution from this study was the refinement of the data for the major oxygen buffer assemblages.

In the geological sciences an increasing use is made of the chemical potential buffers of oxygen as a tool in research. The fugacity of oxygen is an important parameter in volcanogenesis, metamorphism, or ore genesis to cite just a few natural processes. The oxidation state of iron and traces of manganese in complex iron-magnesium aluminosilicates such as chlorites, epidotes, garnets, or pyroxenes control the stability of the solid solutions. The oxidation state also controls the positions of the stability tie-lines with other minerals and with the coexisting fluids or melts. Researchers attempt to deduce the fugacity of oxygen or the changes in the fugacity of oxygen in time and space from the mineral assemblages and the available thermodynamic data for these minerals. The thermodynamic data were derived from laboratory studies. In the research on the stability of complex mineral assemblages containing iron, manganese, or other elements with two or more valence states, the assemblages are equilibrated with simple solid assemblages such as quartz (SiO_2), fayalite (Fe_2SiO_4) and magnetite (Fe_3O_4). Because the chemical potential of O_2 for this assemblage is fixed at a given temperature and pressure by the reaction

$$2\ Fe_3O_4(\text{magnetite}) + 3\ SiO_2(\text{quartz}) = 3\ Fe_2SiO_4(\text{fayalite}) + O_2(g) \qquad 1.1$$

the chemical potential of oxygen in the assemblage is "known". Or is it? Figure 1.1 shows a sample of published equations for the fugacity of oxygen calculated from the equilibrium constant for reaction 1.1. The graphed curves were cited in publications since 1980. If the chemical potential of oxygen for the buffer assemblages are to be used as "known" values, agreement should be better.

Figure 1.1 near here.

This report presents the results of a critical review of the data for these nine oxygen buffer assemblages:

(1) copper(Cu) - cuprite(Cu_2O)

(2) cuprite(Cu_2O) - tenorite(CuO)

(3) nickel(Ni) - bunsenite(NiO)

(4) iron(Fe) - wustite($Fe_{1-y}O$)

(5) iron(Fe) - magnetite(Fe_3O_4)

(6) iron(Fe) - quartz(SiO_2) - fayalite(Fe_2SiO_4)

(7) wustite($Fe_{1-y}O$) - magnetite(Fe_3O_4)

(8) magnetite(Fe_3O_4) - quartz(SiO_2) - fayalite(Fe_2SiO_4)

(9) magnetite(Fe_3O_4) - hematite(Fe_2O_3)

In conducting the critical review, every attempt was made to insure that the recommended chemical potentials of oxygen for the buffer assemblages were consistent with all aspects of the chemical systems. This included analyses of the heat capacities, relative heat contents, and entropies for each of the phases in the system and of the reactions and electrochemical potential data measured either independently of or relative to each other. Volumetric data for the solid phases were also included because many applications require that chemical potentials be known to pressures in excess of 30 kilobars.

A thesis was set up that stated (1) there were sufficient experimental data already in the public literature, and (2) better results would be obtained if a diligent application of thermodynamic theory were applied to these published data. In performing the analysis no experimental research was undertaken. Only published data and thermodynamic principles were used to develop the recommended tables. The revised optimization routine of Haas and Fisher (1976) was used to find the right combination of entropies, enthalpies of formation and thermal functions that produced the best fit of the experimental data within the precision of all data. As an additional benefit of the critical review, the thermodynamic properties of the oxides have been updated.

Acknowledgements

(Paragraphs will be written after all reviews.)

CHAPTER 2

NOMENCLATURE, SYMBOLS, AND CONSTANTS

Table 2.1 supplies the reader with the symbols and abbreviations used in this report. In general, every attempt was made to conform to common useage.

The user will note that phases were cited by mineral name rather than by chemical formula. A chemical formula by itself does not identify the structural state, whereas a mineral name usually is unique to a structural state of a chemical component. If no mineral name existed, that is if the pure chemical composition does not occur naturally, the formula is followed by either (s), (l), or (g) to identify the state. For metallic iron, the identifiers alpha and gamma were used. In this report, Fe(alpha) is equivalent to all of the following: Fe(alpha), Fe(alpha'), Fe(beta), and Fe(delta) as used in other reports. With the fitting functions that were developed here, no additional distinctions were necessary for the body-centered cubic structural state for iron. Also for nickel, Ni(alpha) is equivalent to Ni(alpha) and Ni(beta), the face-centered cubic phase stable below and above the Curie temperature, respectively.

Table 2.2 contains the critical constants and conversion factors used in this report.

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.

Tables 2.1 and 2.2 near here.

CHAPTER 3

SCOPE OF EVALUATION

Introduction

To describe one or maybe two thermodynamic quantities of a chemical system by simple algebraic equations is not an adequate description of the chemical buffer system. A proper analysis examines all available data for the thermodynamics of the system and makes the maximum use of the interrelations among the thermodynamic quantities such as heat capacity, entropy, molar volume, Gibbs energy, and so forth. Such an analysis might be considered "overkill", but it is necessary if the best values for the chemical buffer system are to be obtained. When the results of the analysis are compatible with the first or second derivatives (changes in entropy and heat capacity or with derivatives of the molar volume) as well as with the measured differences among buffer systems, the opportunity for arriving at erroneous conclusions becomes small, indeed.

Phases and Oxygen Buffers Included in Study

In this study, an attempt was made to evaluate the available data for the oxygen buffer assemblages in the copper-oxygen, nickel-oxygen, and iron-silicon-oxygen systems. The desired result should be recommended values for the oxygen buffers when they are used as "yardsticks" to measure the chemical potential of oxygen in other assemblages and solid solutions. The following buffer reactions were included in this evaluation:

$$2\ Cu(s) + 0.5\ O_2(g) = Cu_2O(\text{cuprite}) \qquad 3.01$$

$$Cu_2O(\text{cuprite}) + 0.5\ O_2(g) = 2\ CuO(\text{tenorite}) \qquad 3.02$$

$$Ni(s) + 0.5\ O_2(g) = NiO(\text{bunsenite}) \qquad 3.03$$

$$(1-y)\ Fe(s) + 0.5\ O_2(g) = Fe_{1-y}O(\text{wustite}) \qquad 3.04$$

$$3\ Fe(s) + 2\ O_2(g) = Fe_3O_4(\text{magnetite}) \qquad 3.05$$

$$\frac{6}{(1-4y)} Fe_{1-y}O(\text{wustite}) + O_2(g) = \frac{2(1-y)}{(1-4y)} Fe_3O_4(\text{magnetite}) \qquad 3.06$$

$$2\ Fe_3O_4(\text{magnetite}) + 0.5\ O_2(g) = 3\ Fe_2O_3(\text{hematite}) \qquad 3.07$$

$$2\ Fe(s) + SiO_2(\text{quartz}) + O_2(g) = Fe_2SiO_4(\text{fayalite}) \qquad 3.08$$

$$3\ Fe_2SiO_4(\text{fayalite}) + O_2(g) = 2\ Fe_3O_4(\text{magnetite}) + 2\ SiO_2(\text{quartz}) \qquad 3.09$$

To succeed in the task, the published literature was searched for the available heat capacities, entropies, molar volumes, expansivities, compressibilities, and reaction data. Special attention was given to "primary" and "secondary" data. The results of other evaluations were read with interest but not given any weight in this study. "Primary" data were defined as the experimental data with only instrumental corrections applied but without conversions to thermodynamic properties. For examples, electrochemical potentials reported as volts were considered "primary" data. "Secondary" data were defined as experimental measurements that were converted to other units using defined (or possibly undefined but assumed) constants or experimental measurements that have been smoothed by curve-fitting. An example of "secondary" data would be a set of calculated fugacities (or activities) of O_2(gas) derived from an electrochemical study using the molar gas constant and the Faraday.

Reference Data Taken From Others Sources

Evaluating every aspect of the chemical system was not the aim of this study. The thermal functions for the elements and for the compounds CO(g), CO_2(g), H_2O(s,l,g), and SiO_2(quartz, cristobalite) were taken from the sources indicated below:

Source	Phases
Cox and others (1987)	Cu(s,l)
Garvin and others (1987)	C(graphite), CO(g), CO_2(g) H_2(g), H_2O(g), O_2(g)
Haar and others (1984)	H_2O(ice, water, steam)
Chase and others (1985)	Fe(alpha,gamma), Ni(s,l)
Hemingway (1987)	SiO_2(alpha-, beta-quartz)
Chase and others (1985)	SiO_2(alpha-, beta-cristobalite)

Iron and nickel have lambda-type anomalies in the heat capacities at 1042 and 631 K, respectively. The anomalies are due to the magnetic disordering with increased temperature for the body-centered cubic or alpha-iron phase and for the face-centered cubic nickel phase. In order to have thermal functions that mimic the true curvature of the experimental data, the 100-kelvin-spaced tabulations of the JANAF Thermochemical Tables (Chase and others, 1985) were supplemented with the experimental data upon which the tabulations were based. Least-squares fitting of the combined data sets are in agreement with both the JANAF Thermochemical Tables and with the experimental data within the precision of the experimental data. The volume functions for iron and nickel were fit as a part of the data evaluation process and will be discussed in Chapter 7. The observations for the alpha-to-gamma inversions of iron as a function of pressure were also included in the final optimization and will also be discussed in Chapter 7.

The thermal functions for alpha- and beta-quartz were based on a recent experimental study and critical review by Hemingway (1987). The values for $\Delta_f H°(298)$ and $S°(298)$ were taken from the CODATA Recommended Key Values for Thermodynamics 1987 (Cox and others, 1987). No corrections were needed as a result of the new work by Hemingway (1987) because the enthalpy of formation was based on solution calorimetry near ambient temperature. The volume functions for alpha- and beta-quartz were based on a least-squares fitting of the data contained in the sources below. Figures 3.1 and 3.2 show the correlations of the fitted function to the data.

Source	Temperature Range	Pressure Range
Ackermann and Sorrell (1974)	298-1373 K	1.01 b
Adams and others (1919)	298 K	0-12 kb
D'Amour and others (1979)	298 K	0-73 kb
Jay (1933)	291-1003 K	1.01 b
Levien and others (1980)	298 K	0-62 kb
Olinger and Halleck (1976)	298 K	33-121 kb
Vaidya and others (1973)	293 K	5-45 kb

Figures 3.1 and 3.2 near here.

The fitted functions are also consistent with the work of Berger and others (1966) between 299 and 931 K except in the vicinity of the crystallographic lambda-type anomaly and first-order transition that occurs between 844 and 848 K. The three observations by Ackermann and Sorrell (1974) between 1473 and 1673 K were not included in the fitted set because there was evidence of inversion to beta-cristobalite. The compressibility of beta-quartz is consistent with the above data and the alpha-to-beta inversions as reported by Yoder (1950), Cohen and Klement (1967), and Koster van Gro~~s~~os and Ter Heege (1973).

No attempt was made to separate out the thermodynamic and volumetric properties of the incommensurate phase that occurs over less than a 1-kelvin range near the alpha-to-beta inversion. There are few applications where the properties of the incommensurate phase would be significant.

The thermal functions for alpha- and beta-cristobalite were based on the JANAF Thermochemical Tables (Chase and others, 1985), the evaluation for quartz, and the measured enthalpy difference between alpha-cristobalite and alpha-quartz at 347 K (Kracek and others, 1953) and between beta-cristobalite and beta-quartz at 970 K (Holm and others, 1967). The inversion temperature has not been observed experimentally because the reconstructive process is slow. The calculated inversion, where the Gibbs energy difference becomes zero, is 1207 K. This is a departure from the inversion temperature of 1079 K given in the JANAF Thermochemical Tables (Chase and others, 1985). The thermal function is about 1,200 J/mol lower than the observations by Richet and others (1982), but the latter author's data for quartz were also high by the same amount (Hemingway, 1986).

The volume functions for alpha- and beta-cristobalite were based on a least-squares fit of the data in the sources below. Figure 3.3 shows the correlations of the fitted function to the data.

Source	Temperature Range	Pressure Range
Berger and others (1966)	298-773 K	1.01 b
Johnson and Andrews (1956)	296-1411 K	1.01 b
Wright and Leadbetter (1975)	573-1473 K	1.01 b

Figure 3.3 near here.

There are no experimental data available for the effect of pressure on the molar volume of cristobalite. Fortunately, all reactions where cristobalite was present were conducted at ambient pressure.

Auxiliary Experimental Data

In addition to the direct observations for the reactions 3.01 through 3.09 given above, and for the properties (such as heat capacity, entropy, or volume) of each of the phases in the reactions, the following data were also used as constraints on the mathematical description of the system.

(1) Data on reactions where the oxygen was replaced either by H_2O and H_2 or by CO_2 and CO in the proper proportions to balance the chemical reaction. An example would be the following reaction:

$$\mathrm{Ni(s)} + \mathrm{CO_2(g)} = \mathrm{NiO(bunsenite)} + \mathrm{CO(g)} \qquad 3.10$$

(2) Electrochemical potentials between two buffer assemblages. An example of the net reaction between the buffers represented by equations 3.03 and 3.04 would be the following:

$$(1-y)\ \mathrm{Fe(s)} + \mathrm{NiO(bunsenite)} = \mathrm{Fe_{1-y}O(wustite)} + \mathrm{Ni(s)} \qquad 3.11$$

(3) Measurements of the variation of the composition of wustite as a function of oxygen fugacity, the ratio of $H_2O(g)$ to $H_2(g)$, or the ratio of $CO_2(g)$ to $CO(g)$.

(4) Measurements of the potential difference between wustite samples of known composition and a buffer assemblage.

No use was made of the aqueous chemistry for copper, nickel, or iron. For copper, the data might be useful because the direct observations for the following reaction are available.

$$\mathrm{Cu(s)} = \mathrm{Cu^{2+}(aq)} + 2\ e^- \qquad 3.12$$

However, for iron and nickel, the properties of the aqueous ions are derived from data for the solids. These indirect observations cannot improve the fitting of the data for the oxides.

Reactions outside of the system defined above were also not included in this study. To do so would also involve the evaluation of the introduced phases. Because such additions are not likely to constrain the results more closely, the study was restricted to the system defined and reactions with other oxides such as CoO, MgO, CaO, and with other more complex silicates were not included.

When the study was originally developed, the oxides of manganese were also included (Haas, 1984). However, as the study developed it was realized that the data for the manganese oxides were of very limited value in fixing the data for the oxygen buffers included here. The data for the manganese oxides have been set aside for a separate evaluation.

Wustite, A Special Problem

Figure 3.4 near here.

The commonly accepted stability relations in the iron-oxygen system are given on Figure 3.4 and are based on estimates and data supplied by Darken and Gurry (1945, 1946). The diagram is given for information only. The results of this review differ in some important details that will be discussed in Chapter 7.

The thermochemistry of wustite has been a special problem for compilers and evaluators of thermodynamic data. Wustite is a solid with a defect NaCl structure. The common formula is $Fe_{1-y}O$ but for some purposes the formula FeO_{1+x} is used. Tabulations are available for $Fe_{0.947}O$ in most compilations of thermodynamic data. Other formula more closely related to the structure are also available. In the above formula, y is the moles of iron deficit, and x is the moles of oxygen excess to the stoichiometric formula, FeO. It is recognized that these formula do not identify all structural complexities. The reader is referred to the recent review by Hazen and Jeanloz (1984) for a more detailed discussion of the solid solution.

The phase wustite contains some excess oxygen at all pressures and all temperatures (Simmons and Seifert, 1979; Liu and others, 1984). Stoichiometric FeO as a metastable intermediate phase of the decomposition of wustite at 225°C and ambient pressure was found by Hentschel (1970). However, the quenched cell dimensions indicated that phase was not stoichiometric. The quenched cell dimensions are smaller than was expected. Hazen and others (1981) reported a non-elastic behavior for wustites held at pressures greater than 150 kb and room temperatures for durations of two weeks or more. Jeanloz and Hazen (1983) attributed the anomalies to diffusion-controlled ordering of defects at elevated pressures. Akimoto's (1972) observation of stoichiometric wustite at elevated pressure and temperature with anomalously lower cell dimensions upon quenching may be reported correctly. The small cell dimensions observed at ambient conditions may be another manifestation of ordering induced at lower pressures than those used by Hazen and others (1981) due to the elevated temperatures.

For practical purposes, the compositions of wustite coexisting with iron or with magnetite are known only poorly. After the early attempts by Chaudron (1921), there have been many studies to define the stability limits and thermodynamic properties of wustite. The attempts have been a mixture of experimental data, theory, and assumptions with varying justifications. Among the more prominent studies were the work of Darken and Gurry (1945, 1946), of Engell (1957), of Vallet and Raccah (1965) and later coworkers, and of Giddings and Gordon (1974).

The establishment of the composition limits of wustite is difficult.

Direct chemical analys~~i~~es have yielded poor results. The compositions were calculated indirectly from the intersections of plots of a property such as electrochemical potential or fugacity of oxygen as a function of composition at constant temperature within the solid solution and plots of the same property measured for the bounding two-phase assemblages as a function of temperature. The most widely quoted values for the compositions of wustite coexisting with iron and magnetite are the results of measurements and estimates by Darken and Gurry (1945, 1946). Refer to Figure 3.4. Based on experimental measurements at and above 1373 K and on published data for gas ratios of CO_2(g) and CO(g) for the two-phase boundaries, Darken and Gurry estimated the compositions down to the disproportionation temperature of 833 K. The estimated composition at 833 K was $Fe_{0.945}O$ (Darken and Gurry, 1946). It must be emphasized here that this composition does not have a direct experimental basis.

The compositional data of Darken and Gurry (1945, 1946) were used by later researchers as guide for the preparation of a wustite sample, $Fe_{0.947}O$, for calorimetry (Coughlin and others, 1951; Humphrey and others, 1952). The method of Blue and Claassen (1949) was used to prepare the sample. The amounts of iron and magnetite needed to make a wustite of known composition were placed at opposite ends of a silica tube. A small amount of water was placed in the tube and the tube sealed without mixing the iron and the magnetite. On heating to 700 to 900°C, the water reacted with the two solids and converted both to wustite. The wustite from the magnetite-end of the silica tube was used by Coughlin and others for their calorimetric studies. Subsequent evaluators tabulated the thermodynamic properties for the composition of the calorimetric sample, $Fe_{0.947}O$, relying on the calorimetric measurements from this sample (heat capacity, relative heat content, entropy, and heat of solution) and on the apparent absence of significant compositional changes for the wustite coexisting with iron as indicated on Figure 3.4. The composition of wustite coexisting with iron on the phase diagram prepared by Darken and Gurry (1945, 1946) varies from $Fe_{0.954}O$ to $Fe_{0.945}O$. In this review, the composition $Fe_{0.947}O$ will be given no special treatment because it has no significance beyond being a sample used in calorimetric studies. It will be shown that the composition of the wustite coexisting with iron varies significantly and the composition of the calorimetric sample is metastable below about 1050 K.

In this study, no assumptions were made a priori except as given in Chapter 5, below. The most critical of those assumptions was that the log of the fugacity of oxygen was a linear function of the amount of excess oxygen, x, in the wustite solid solution, where FeO_{1+x} was used as the chemical formula. The thermodynamic properties were evaluated and tabulated for stoichiometric FeO and for wustites with y varying from 0.00 to 0.16, where $Fe_{1-y}O$ was used as the chemical formula. The terms x and y have the following relationship to each other:

$$1 - y = \frac{1}{1 + x} \qquad 3.13$$

Vallet and coworkers (See Vallet and Carel, 1979) have proposed the existence of sub-domains within the wustite stability limits. It is not clear whether the sub-domains are separated by first-order transitions or by second-order transitions and the authors are not clear on that point with the phase diagrams that they present. In part, some of the diagrams violate the phase rule for a two-component system at constant pressure. Other authors have not succeeded in reproducing the same results or have found results that were not compatible with the existence of the sub-domains (Giddings, 1972; Hayakawa and others, 1972; Touzelin, 1974). In this analysis the existence of sub-domains was considered but the phenonemon was not used in the refinement process. As suggested by Hazen and Jeanloz (1984), a more detailed study of the factors time, temperature, pressure, and transformation should be made before real progress in the development of a detailed thermodynamic description of wustite would be possible. At this time, such a description must be left for the future when the careful work needed for such an analysis is completed. In doing the careful work, the researcher must record the composition and the structural state of the phases both before and after the experiments. As will be pointed out in Chapter 11, Recommendations for Future Research, the observations of transient phenomenon during the experiments will also be important.

The review for wustite, as presented here, will differ greatly from all previous reviews. For example Spencer and Kubaschewski (1978) and Esdaile (1983) accepted all results from the studies by Darken and Gurry (1945, 1946) without further critical review. This included accepting the values derived from extrapolations over a temperature range as large as 500 kelvin. Knacke (1983) used additional data derived from the study by Giddings and Gordon (1974) but made no attempt to conduct a thorough review of data or to apply all available thermodynamic constraints to the wustite solid solution and to the chemical relations among wustite, iron, and magnetite. In this study, only experimental observations or reasonable inferences based upon observations were considered. As stated before, the results of reviews were not included. The reviews (Chase and others, 1985; Leonidov and Medvedev, 1984, and others), however, were read with interest. The tests for validity of this evaluation was not how well it agreed with previous reviews but how well the experimental data could be calculated using the mathematical model developed in the evaluation.

Literature Searched

The published literature was searched through December, 1986. Emphasis was placed on obtaining copies of the papers and only minor effort was given to data available only in an abstract. Data that were available as points or curves on a graph generally were ignored. This course of action was based upon the belief that scaling data from a graph most often gave results that were inferior in precision to other data that were precisely reported. Examples would be the heat capacity measurements on NiO, bunsenite, by Lewis and Saunders (1973) or by Mainard (1963), or on Fe_3O_4, magnetite, by Shepherd and others (1985). Apparently, the authors did not recognize their results as being either important enough or accurate enough to supply the data for their measurements made up to 640 K. The net result was that the measurements for NiO were repeated recently by Hemingway (1984).

Some studies were rejected upon first reading because the data supplied by the study had to be in error. An example would be the study by Choi and others (1973) where they report the coexistence of wustite solid solution with oxygen gas pressures varying from 10^{-4} to 100 mm Hg and wustites varying from FeO to $Fe_{0.112}O$. These results are not consistent with any other studies in the published literature. Another example is the work by Janowsky and others (1974). Refer to Figure A.21, part n in Appendix A.

CHAPTER 4

METHOD OF EVALUATION

In conducting the evaluation, all experimental data related to chemical reactions given in Chapter 1 were collected and reviewed. Other reviews were read but were not used, except that they supplied insight into various aspects of the data set. As with previous evaluation techniques, least-squares fitting of data were performed both to identify conflicts and to smooth the data, but, unlike other approaches, these fittings were performed simultaneously on all properties of a phase and all interactions among phases. In order to accomplish this, the mathematical model for the properties of the phases in the buffer system was developed. The functions are given in Chapter 5.

It is not possible to begin the least-squares fitting on the complete data set as the first step. If this were tried, overfitting or underfitting of data would occur because one does not always know how many and which algebraic terms should be included for each phase. Preliminary least-squares fitting of the data for heat capacity, specific heat, and relative heat content (incremental enthalpies) were made to identify the appropriate constants and to eliminate the non-significant constants. The same was done for fitting the volume-related data. ~~T~~When these steps were completed for each phase, all data for all phases and for all interactions among the phases were evaluated using the least-squares approach described below. In the this final step only the terms that were found to be significant were allowed to be fit to the data. The other terms were constrained to be zero.

An extension of the least-squares procedure of Haas and Fisher (1976) was used to develop the final optimization. The method performs simultaneous, least-squares fitting of a set of related functions in a mathematical model to the measured properties of each phase in the chemical system and to the observed chemical reactions and electrochemical potentials among groups of phases in the system. The mathematical model used in this study is supplied in Chapter 5. There are several features that make this approach useful for the evaluation of mineral thermodynamics:

(1) The approach is phase-oriented and not composition-oriented. The method is readily adaptable to evaluating both stable and metastable equilibria because the phase and not the composition is specified.

(2) The method allows for fitting of isochemical inversions among phases. Where the temperature of a polymorphic inversion is known within narrow limits (e.g. 5 K), the method forces the Gibbs energy difference between the two polymorphs to be zero at the inversion temperature and the reference pressure. If the temperature of an inversion is unknown or only poorly known (±25 kelvin), the inversion temperature can be determined after the optimization. An example of a well defined invers~~t~~ion temperature would be the first-order phase change between ice and water at 273.15 K and 1 bar. With this feature, it was relatively easy to evaluate the thermodynamic data associated with alpha- and gamma-iron or with any other polymorphic series.

(3) The method allows for weighting of the data. An attempt was made to fit all observations within the precision of the observations. For precision, the experimentor's estimate was used except for those

observations where the precisions were found to be excessively small in absolute magnitude. In those situations, the precision was revised to reflect the scatter in the set of observations or to reflect the inherent imprecision in the method or both. The weighting factor W of each observation was set as follows:

$$\underline{W} = \frac{1}{(\text{precision})^2} \qquad 4.1$$

where the precision was an absolute quantity and was expressed in the same units as the observation. Where the data were believed to be in error, a weight of "zero" was given by setting the precision to 10^{15}.

(4) The method allows for the optimization of different but related properties for a phase without separate fittings. A simple example would be the simultaneous fitting of data for C_p, H(T)-H(298), and S(298) for a phase. By being able to fit the mathematical model to the complete spectrum of experimental data simultaneously, the agreement or discordance of the data was immediately apparent.

(5) The method is readily expandable to include additional variables. The procedure originally described by Haas and Fisher was expanded to allow for two additional independent variables for a total of four independent variables. In this study, the additional independent variables were the pressure of the observation and a reference pressure or, alternately, the composition x of the wustite phase where FeO_{1+x} was used for the formula for that phase.

(6) The method has the capability of fitting functions that are non-linear in the constants. This was necessary to be able to fit expansivity and compressibility data and a considerable body of data related to the

thermochemistry of wustite.

(7) The method allows for the insertion of additional constraints through the user-defined subroutines. This feature was necessary to derive the most benefit from the observations where wustite was present. The observations, either fugacities of oxygen, ratios of H_2O to H_2 or of CO_2 to CO, electrochemical potentials, or compositions from coulometric titrations, could be calculated from the equilibrium constants and the corrections for the activity of Fe or FeO in the solid solution where the composition was known.

(8) The procedure is expandable to evaluate the properties of many phases and to consider large numbers of observations by simple changing of dimensions in the computer code. In this problem, about 40 phases were included, but this number may be expanded to greater than 150. Many of these were phases with fixed properties that were derived from previous work by the CODATA Task Groups. Over 8,000 observations were included in the final evaluation.

(9) The method allows for the trial fitting of the experimental data where S°(0), the entropy at the absolute zero of temperature, for a phase might be set to some theoretical value. S°(0) can also be a fitted constant where the term takes on the value necessary to produce the least-squares minimum in the regression process.

(10) Finally, because the method involves a regression analysis, the preparation of tables of properties that includes a statistically-derived 2-sigma confidence limit on the predicted properties is possible. Hence the tables to be presented in a later chapter will include such 2-sigma confidence limits at each 250-K isotherm.

The successful use of the method does depend upon many human factors.

Among them is the diligence with which the experimentalists explored the physical phenomenon and published objective descriptions of the experimental observations. These are beyond the control of the evaluator. At this point it would also be stated that the policy of many journals influenced the quality of the published data. Some journal editors erroneously limit an author's freedom to publish by permitting the printing of graphs that are too small for scaling of data or by permitting equations that smooth and bias the data and do not match the detail that is present in the experimental data.

Where possible, authors were contacted for a table of experimental data. This evaluator greatly appreciates the cooperation supplied by W.W. Smeltzer, S.N. Flengas, Mats Hillert, J. Myers, R.M. Hazen, B.S. Hemingway, Erik Rosen, H.P. Eugster, N.B. Neskovic, P. Chiotti, and A. Trumm. The user of this compilation owes a debt of thanks to them for their cooperation. The user should also complain strongly when an editor wishes to denigrate their research effort by reducing or removing the experimental facts that are the very basis of their report.

There was also the diligence with which this evaluator searched the literature and abstracted the quantitative data, assigned weights to the data and sought a solution that objectively reproduced the data. It is hoped that little can be found that this evaluator did not include in attending to the task.

CHAPTER 5

FUNCTIONS DESCRIBING THERMODYNAMIC PROPERTIES

Introduction

In order to use a least-squares approach to correlate experimental measurements of thermodynamic properties of all types, it is mandatory that explicit algebraic functions exist that relate all properties to each other. By the same token, if an experimental observation can be calculated from thermodynamic data, the experimental observation can be used as a constraint on the thermodynamic properties in a least-squares evaluation procedure. In this chapter, the functions were derived to fit the heat capacity, entropy, enthalpy, Gibbs energy and molar volume of every phase, and the enthalpies of reaction, Gibbs energy changes, equilibrium constants, and electrochemical potentials for reactions among a group of phases. For wustite ($Fe_{1-y}O$ or FeO_{1+x}), the functions that relate the molar volume, the logarithms of the activity of FeO, Fe, and O_2 to the composition of the wustite solid solution were also developed. In turn, the composition of the wustite coexisting with iron or with magnetite as well as the compositional width of the wustite stability field were also derived from these equations. In setting up the mathematical model used in this analysis, only a minimum of empirical assumptions were developed. To the extent possible, the maximum use was made of the interrelations among the thermodynamic properties. In addition, the Fe-O system allowed the use of some special constraints.

The model, using an integrated set of algebraic representations that do not violate thermodynamic theory, makes possible the analysis of a broad spectrum of data. The primary purpose of the model is served within the scheme of data analysis and in the optimization of the thermodynamic properties for the chemical system being evaluated. The details are being presented here to allow the reader an understanding of the approach to this task. The model is not presented with the aim that it be adopted for general useage though this author has found the model equations useful for subsequent thermodynamic predictions.

General Thermodynamic Relationships

At constant bulk composition, thermodynamic theory provides the following exact functional relations among temperature (T), volume (V_i), coefficient of volume expansion (alpha_i), coefficient of volume compression (beta_i), heat capacity ($C_{Pr,i}$) at a reference pressure Pr, the heat capacity ($C_{P,i}$) at an arbitrary pressure P, volume (V_i), entropy (S_i), Enthalpy (H_i), free energy or Gibbs energy (G_i), equilibrium constant (K), and electrochemical potential (E):

$$\mathrm{alpha}_i = \frac{1}{V_i} \frac{\delta V_i}{\delta T}_P \qquad 5.01$$

$$\mathrm{beta}_i = -\frac{1}{V_i} \frac{\delta V_i}{\delta P}_T \qquad 5.02$$

$$C^{\circ}_{P,i} - C^{\circ}_{Pr,i} = -\int_{Pr}^{P} T \, (\delta^2 V_i / \delta T^2 {}_P) \, dP \qquad 5.03$$

$$S_i^\circ = S_i^\circ(0,Pr) + \int_0^T (C_{Pr,i}^\circ/T)\, dT - \int_{Pr}^P (\delta V_i/\delta T|_P)\, dP \qquad 5.04$$

$$H_i^\circ = H_i^\circ(Tr,Pr) + \int_{Tr}^T C_{Pr,i}^\circ\, dT + \int_{Pr}^P [V_i - T(\delta V_i/\delta T|_P)]\, dP \qquad 5.05$$

$$G_i = H_i - T S_i \qquad 5.06$$

$$-R\,T \ln K = \sum_{i=1}^{j} n_i G_i \qquad 5.07$$

$$-n_e F E = \sum_{i=1}^{j} n_i G_i \qquad 5.08$$

where R and F are the ideal gas constant and the Faraday constant, respectively. Tr is a reference temperature (kelvin) for the enthalpy or Gibbs energy. For practical purposes, Tr is 298.15 K in this evaluation. The restriction on Tr is that the function for $C_{Pr,i}$ and V_i include Tr within the range of validity for the function. The term j is the number of species in the reaction and n_i is the stoichiometric coefficient for the ith species, positive for each product and negative for each reactant. The term n_e is the number of electrons involved in the reaction.

In all subsequent notation, the enthalpy and Gibbs energy of a phase will be identified by h_i and g_i, respectively. The intention is to identify these terms and show that they depart from common useage. Where the symbols H and G are used, they will refer to standard IUPAC notation (Commission on Thermodynamics, 1982).

Reference States

In using equations 5.01 through 5.08, two reference states were identified. They were $S_i^\circ(0,Pr)$ and $h_i^\circ(Tr,Pr)$.

$S_i(0,Pr)$ refers to the residual entropy at the absolute zero of temperature. In practice, the mathematical model contains a constant of integration $a_{10,i}$ that is fit during the regression analysis of all data including the supplied data for $S^\circ(T)-S^\circ(0)$, if any. If a zero-point entropy were to be considered, the magnitude of the zero-point entropy would be either added to the data set or forced to be an estimated value and added onto the calculated entropy during the fitting procedure.

The reference temperature Tr for enthalpy, $h_i^\circ(Tr,Pr)$, was set to 298.15 K. For all elements in their stable structural state at 298.15 K, $h_e^\circ(298,Pr)$ was set equal to the quantity $298.15 \cdot S_e^\circ(298,Pr)$ where $S_e^\circ(298,Pr)$ was the entropy of the reference structural state at 298.15 K and Pr. From this identity, it followed that $g_e^\circ(298,Pr)$ for all elements was zero at 298.15 K (equation 5.10). It also followed that the Gibbs energy for other phases at 298.15 K was identical to the Gibbs energy of formation from the elements at 298.15 K and the reference pressure.

$$h_e^\circ(298,Pr) = 298.15 \cdot S_e^\circ(298,Pr) \qquad 5.09$$

$$g_e^\circ(298,Pr) = 0 = h_e^\circ(298,Pr) - 298.15 \cdot S_e^\circ(298,Pr) \qquad 5.10$$

The chosen state permitted use of terms in the empirical equation for heat capacity that would become undefined at T = 0 kelvin and gave a better mathematical description of the heat capacity data. The chosen state also made programming of the mathematical model less complex. In practice, $h_i^\circ(Tr,Pr)$ and the residual when equation 5.05 was evaluated at 298.15 K were combined into one fitted constant of integration, $a_{9,i}$.

The convention used in the fitting of enthalpy and Gibbs energy differs from standard conventions in that a single reference state at a specific temperature and pressure was used. That reference temperature and pressure was 298.15 K and 1 atm (1.01325 bar), respectively. Gibbs energy and enthalpy are related to standard notation as follows:

$$g_i^\circ(T,P) = \Delta_f G_i^\circ(298K,1.01\ b) + \int_{298}^{T} S_i^\circ\, dT + \int_{1.01}^{P} V_i^\circ\, dP \qquad 5.11$$

$$h_i^\circ(T,P) = g_i^\circ(T,P) + T \cdot S_i^\circ(T,P) \qquad 5.12$$

In order to conform with current useage, the evaluated results were converted from the one-atm reference state used in the evaluation to the one-bar reference state prior to the generation of the tables that are presented in later chapters.

Empirical Equations Describing the Thermodynamic Relations

From the relations given in the preceding section, it follows that an empirical equation that describes the heat capacity $C_{Pr,i}$ as a function of temperature and the volume V_i as a function of temperature and pressure will generate the mathematical description for the thermodynamic properties. The empirical functions and the equations for other properties generated from them are given in the following sections.

Empirical Equation for the Molar Volume of a Phase as a Function of Pressure and Temperature

The molar volume of a phase was fit using the following function (modified from Robinson and others, 1983):

$$V_i = [b_{1,i} + b_{2,i}T + b_{3,i}e^{(-T/300)}]\cdot[1 + b_{4,i} + b_{5,i}e^{(-P/35000)}] \qquad 5.13$$

Equation 5.13 gives the molar volume as a function of temperature and pressure. The experimental data, presently available, can be adequately fit with such a function, but this was because measurements were made either at one atmosphere (nominal) and elevated temperature or at room temperature (293 or 298 K, nominal) and elevated pressure. As data become available, additional terms can be added. The first exponential term mimics the expansivity curve for a solid. The second exponential term mimics the compressibility curve of a solid. The use of these exponential terms eliminated the extreme excursions that would be possible from a simple power series. Figures 5.1 and 5.2 are examples of the fitting of the above function to the data for bunsenite, NiO.

Figures 5.1 and 5.2 near here.

Coefficient of Volume Expansion of a Phase

From equation 5.13, equations for several types of data, as reported in the literature, were derived. The coefficient of volume expansion was:

$$\mathrm{alpha}_i = \frac{1}{V_i} \frac{\delta V_i}{\delta T}_p \qquad 5.14$$

$$\mathrm{alpha}_i = \frac{b_{2,i} - \frac{b_{3,i}}{300} e^{-T/300}}{b_{1,i} + b_{2,i}T + b_{3,i}e^{-T/300}} \qquad 5.15$$

Experimental data are usually reported as volume differences relative to a reference volume at a reference temperature.

$$\text{"alpha"}_i = \frac{1}{Vr_i} \frac{V_i - Vr_i}{T - Tr}_p \qquad 5.16$$

where Vr_i is the reference volume at Tr. The model equation for this observation was

$$\text{"alpha"}_i = \frac{b_{2,i}(T-Tr) + b_{3,i}(e^{-T/300} - \exp^{-Tr/300})}{b_{1,i} + b_{2,i}Tr + b_{3,i}e^{-Tr/300}} \cdot \frac{1}{(T-Tr)} \qquad 5.17$$

Figure 5.3 shows the plot of the coefficient of volume expansion as a function of temperature for fayalite, Fe_2SiO_4.

Figure 5.3 near here.

Coefficent of Volume Compression of a Phase

In like manner, the coefficient of (volume) compression is

$$\text{beta}_i = -\frac{1}{V_i}\frac{\delta V_i}{\delta P}_T \qquad 5.18$$

$$\text{beta}_i = -\frac{b_{4,i} - \frac{b_{5,i}}{35000}e^{-P/35000}}{1.0 + b_{4,i}P + b_{5,i}e^{-P/35000}} \qquad 5.19$$

In the empirical equation, beta_i is independent of temperature. The optimization produces an average beta_i. For iron the function has been adequate within the precision of the data to fit the data to 700 kb and 873 K (600°C).

Again, experimental data are usually reported as volume differences relative to a reference volume at a reference pressure. Then

$$\text{"beta"}_i = -\frac{1}{Vr_i}\,\frac{V_i - Vr_i}{P - Pr}_T \tag{5.20}$$

where Vr_i is the reference volume at Pr. The model equation for this observation was

$$\text{"beta"}_i = -\frac{b_{4,i}(P-Pr) + b_{5,i}(e^{-P/35000} - e^{-Pr/35000})}{1.0 + b_{4,i}Pr + b_{5,i}e^{-Pr/35000}} \cdot \frac{1}{(P-Pr)} \tag{5.21}$$

Empirical Equation for the Heat Capacity of a Phase at Constant Pressure

Empirically, it was found that the following function will describe the heat capacity for most phases as a function of temperature T at a constant pressure Pr.

$$C_{Pr,i} = a_{1,i}\,T^{-3} + a_{2,i}\,T^{-2} + a_{3,i}\,T^{-1} + a_{4,i}\,T^{-.5} + a_{5,i} + a_{6,i}\,T + a_{7,i}\,T^{2} + a_{8,i}\,T^{3} + C_{M,i} \qquad 5.22$$

The last term, $C_{M,i}$, is necessary for phases that have second-order magnetic anomalies such as magnetite. They will be discussed later.

All too often a "curve fitter" will attempt to use all terms and then complain in print that the empirical function violates thermodynamic theory. The real violation was the author's blind use of least-squares procedures without any consideration for the significance of the fitted constants. No phase has a complex heat capacity that requires use of all fitting terms given in this equation. In order to avoid overfitting of the available data for a phase, attention was paid to the significance of each constant. For most phases, the second through sixth terms are more than adequate. The other terms are included 1) because other authors have employed them, and 2) their useage may be desir~~e~~able in some situations. In the above equation, the second, fifth and sixth terms are the same as in the classical Maier-Kelley equation for heat capacity (Maier and Kelley, 1932). The second, fourth, fifth, sixth, and seventh terms are the same as those used by Haas and Fisher (1976) and by Robie and others (1979).

The first, second, fourth, and fifth terms of equation 5.22 are used by Berman and others (1984, 1985) to represent the heat capacity of silicates. To eliminate unreliable extrapolations at high temperatures, Berman and others recommended that the second and fourth constants must be less than or equal to zero.

Fei and Saxena (1987) recently proposed the following equation for the heat capacity that incorporates the Petit-Dulong limit for C_V, and the conversion of C_V to C_P:

$$C_P = 3 R n (1 + k_1 T^{-1} + k_2 T^{-2} + k_3 T^{-3}) + (A + B T) + C_P' \qquad 5.23$$

The first term to the right of the equality refers to the Petit-Dulong limit for C_V. The term (A + B T) is an approximation for the quantity alpha^{2}VT/beta. The last term, C_P°, was added to cover departures from the Petit-Dulong limit for those substances that exhibit disordering, anharmonic, mangetic, and electronic contributions to the heat capacity. The above function may be mapped into equation 5.22 above. However, in this study, this equation was not used. Use was made of the Petit-Dulong limit for heat capacity and that will be discussed below.

Where possible, unreliable extrapolations or maxima in the heat capacity function were eliminated by choice of fitting terms on an <u>ad hoc</u> basis. In certain intractable situations, where no combination of terms leads to proper fits of the high temperature data, the Dulong-Petit limit and the relation between $C_{V,i}$ and $C_{P,i}$ were employed:

$$C_{P,i} = C_{V,i} + (V_i \ \text{alpha}_i^2 \ T)/\text{beta}_i \qquad 5.24$$

where $C_{V,i}$ is the heat capacity at constant volume. The terms $alpha_i$ and $beta_i$ are the coefficients of volumetric expansion and of volumetric compression of the phase, and are calculated from equations 5.10 and 5.14, respectively. For practical purposes, where the temperature is several times greater than the Debye characteristic temperature, θ_D, $C_{V,i}$ is approximately equal to (3 R m) where m is the total number of moles of atoms in the formula. The heat capacity at constant pressure was estimated at a temperature at least 3 times the Debye temperature and used as an an "observation". In practice, the temperature usually was 2000 K or higher.

Certain phases have lambda anomalies associated with Neel temperatures, Curie temperatures or other second order phenomena where the phase undergoes changes in the orientation of the magnetic structure. Measured heat capacities of such phases have a cusp and cannot be fit by the generalized function for $C_{p,i}$. An example using the experimental data for bunsenite (NiO) is given in Figure 5.4.

Figure 5.4 near here.

Hillert and Jarl (1978) approximated the magnetic portion of the anomaly by the following functions. For temperatures less than or equal to the critical temperature, where the critical temperature is the temperature of the maximum in the anomaly

$$C^{\circ}_{M,i} = kappa^{a}_{i} R \ln (1 + tau^{3})/(1 - tau^{3}) \qquad 5.25$$

For temperatures greater than the critical temperature,

$$C^{\circ}_{M,i} = \mathrm{kappa}^{b}_{i} \, R \ln (\mathrm{tau}^{5} + 1)/(\mathrm{tau}^{5} - 1) \qquad 5.26$$

The quantity tau is defined as T/T_C. The terms kappa^{a}_{i} and kappa^{b}_{i} are two constants for the ferromagnetic (a) and paramagnetic (b) states of the ith phase. The powers 3 and 5 are empirical. In this study, where these powers were not adequate they were set by visual inspection of the plots from various fittings of the function to the available experimental data.

Following the approach of Agren (1979), the logarithms were replaced by the following MacLauren expansion. For temperatures less than or equal to the critical temperature,

$$C^{\circ}_{M,i} = 2 \, \mathrm{kappa}^{a}_{i} \, R \sum_{k=1}^{n} \mathrm{tau}^{j'_{i}(2k-1)}/(2k-1) \qquad 5.27$$

For temperatures greater than the critical temperature,

$$C^{\circ}_{M,i} = 2 \, \mathrm{kappa}^{b}_{i} \, R \sum_{k=1}^{n} \mathrm{tau}^{j''_{i}(2k-1)}/(2k-1) \qquad 5.28$$

In this study, the temperature T_C were adjusted somewhat to give the best fit of the available data. The values used in this study are somewhat higher than the reported values but generally not by more than 2 kelvin. The critical temperature, T_C, was calculated from the list of constants using the following equation:

$$T_{C,i} = a_{11,i} + a_{12,i}(P-1.01325) \qquad 5.29$$

The series was usually truncated at k = 7 but was extended to k = 15 for the elements iron and nickel. As stated above, the powers j_i' and j_i'' were obtained by visual inspection of plots of the experimental data and trial fittings of the functions.

In this study, 5 phases, the properties of which were being evaluated, and 2 elements had lambda anomalies within or close to the temperature range of 200 to 1800 K. The phases and the critical temperatures are given on Table 5.1.

Table 5.1 near here.

Acceptable past procedures for fitting thermochemical data allowed for the fitting of the heat capacity data and heat content data as well as possible and substituting the algebra for a first-order inversion to mimic the heat capacity curve for the second-order lambda anomaly. By using equations 5.27 and 5.28 this was no longer needed. The complete equations for the heat capacity of the phases listed on the table are given below. For temperatures less than or equal to the critical temperature,

$$C_{Pr,i} = a_{1,i} T^{-3} + a_{2,i} T^{-2} + a_{3,i} T^{-1} + a_{4,i} T^{-.5} + a_{5,i} + a_{6,i} T + a_{7,i} T^{2} + a_{8,i} T^{3} + a_{13,i} \sum_{k=1}^{n} \frac{tau^{j'_i(2k-1)}}{2k-1} \qquad 5.30$$

For temperatures greater than the critical temperature,

$$C_{Pr,i} = a_{1,i} T^{-3} + a_{2,i} T^{-2} + a_{3,i} T^{-1} + a_{4,i} T^{-.5} + a_{5,i} + a_{6,i} T + a_{7,i} T^{2} + a_{8,i} T^{3} + a_{14,i} \sum_{k=1}^{n} \frac{tau^{j''_i(2k-1)}}{2k-1} \qquad 5.31$$

where j'_i and j''_i were empirical coefficients selected by trial, and n was 7 for for the oxides in this study. For iron and nickel, the exponents were +3 and -5, respectively to conform with useage elsewhere. For these elements n was set to 15. In these equations, the constants (2 kappa^{a}_{i} R) and (2 kappa^{b}_{i} R) were replaced by fitted parameters $a_{13,i}$ and $a_{14,i}$, respectively.

Figure 5.4 shows the fit to the heat capacity data of bunsenite, NiO. The solid line was calculated from the fitted constants and equations 5.30 and 5.31, above. These data will be supplied in a later chapter.

Equations 5.30 and 5.31 are continuous at tau = 1 only if $a_{13,i}$ = $a_{14,i}$. In this study, as in the earlier studies (Agren, 1979; Fernandez Guillermet and Gustafson, 1984), these constants were not constrained to be equal. Figure 5.5 is an enlarged portion of Figure 5.4 near 519 K. The error in calculated heat capacities is small and not significant relative to the precision of the data. However, because the constants are not identical, corrections were introduced to force entropies, enthalpies, and other properties derived by integration to be identical at the temperature of the anomaly. The corrections are constants, being only a function of the two fitted constants $a_{13,i}$ and $a_{14,i}$, the exponents j_i' and j_i'', the critical temperature T_C, and the nth term at which the series is truncated.

Figure 5.5 near here.

Entropy of a Phase

After integration of the heat capacity functions (equations 5.30 and 5.31) and using the relation given in equation 5.04, the entropy functions at temperature and pressure for a phase is given by equation 5.32, below.

$$S^\circ_i = S^\circ_i(0) - \frac{a_{1,i}}{3\,T^3} - \frac{a_{2,i}}{2\,T^2} - \frac{a_{3,i}}{T} - \frac{2\,a_{4,i}}{T^{.5}}$$

$$+ a_{5,i} \ln T + a_{6,i}\,T + a_{7,i}T^2/2 + a_{8,i}\,T^3/3 + a_{10,i}$$

$$+ S^\circ_{M,i} - \int_{Pr}^{P} \frac{\delta V}{\delta T}\,dP \qquad 5.32$$

For all phases without a lambda-type anomaly, $S^\circ_{M,i}$ is zero. For a phase with a lambda-type anomaly and at temperatures less than the critical temperature,

$$S^\circ_{M,i} = a_{13,i} \sum_{k=1}^{n} \frac{tau^{j'_i(2k-1)}}{j'_i(2k-1)^2} \qquad 5.33$$

For a phase with a lambda-type anomaly and at temperatures greater than the critical temperature,

$$S^{\circ}_{M,i} = a_{14,i} \sum_{k=1}^{n} \frac{tau^{j''_i(2k-1)}}{j''_i(2k-1)^2}$$

$$+ \; a_{13,i} \sum_{k=1}^{n} \frac{1}{j'_i(2k-1)^2} \; - \; a_{14,i} \sum_{k=1}^{n} \frac{1}{j''_i(2k-1)^2} \qquad 5.34$$

The integral in equation 5.32 is given by the following equation.

$$\int_{Pr}^{P} \frac{\delta V}{\delta T} \, dP = [b_{2,i} - \frac{b_{3,i}}{300} e^{(-T/300)}] \cdot$$

$$(P-Pr) + \frac{b_{4,i}}{2}(P^2-Pr^2) - 35000 \, b_{5,i} \, [e^{(-P/35000)} - e^{(-Pr/35000)}]$$

$$5.35$$

Without specific evidence that $S^{\circ}_i(0)$ differed from zero, the first approach was to assume that $S^{\circ}_i(0)$ was zero. For the phases evaluated and the data used in this study, the assumption produced an acceptable fit.

Enthalpy of a Phase

The equations below give the enthalpy of the ith species at temperature and pressure.

$$h_i^\circ = -\frac{a_{1,i}}{2\,T^2} - \frac{a_{2,i}}{T} + a_{3,i}\ln T + 2\,a_{4,i}\,T^{.5} + a_{5,i}\,T + a_{6,i}\frac{T^2}{2} + a_{7,i}\frac{T^3}{3} + a_{8,i}\frac{T^4}{4} + a_{9,i} + h_{M,i}^\circ + \int_{Pr}^{P} V\,dP - T\int_{Pr}^{P}\frac{\delta V}{\delta T}\,dP \qquad 5.36$$

For all phases without a lambda-type anomaly, $h_{M,i}^\circ$ is zero. For a phase having a lambda-type anomaly and at temperatures less than or equal to the critical temperature,

$$h_{M,i}^\circ = a_{13,i}\sum_{k=0}^{n}\frac{T_C\ \mathrm{tau}^{j_i'(k'+1)}}{k'(j_i'k'+1)} \qquad 5.37$$

where k' = 2k-1. For a phase having a lambda anomaly and at temperatures greater than the critical temperature,

$$h^{\circ}_{M,i} = a_{14,i}\sum_{k=0}^{n} \frac{T_C\ tau^{j''_i(k'+1)}}{k'(j''_i k'+1)}$$

$$+\ a_{13,i}\sum_{k=0}^{n} \frac{T_C}{k'(j'_i k'+1)} - a_{14,i}\sum_{k=0}^{n} \frac{T_C}{k'(j''_i k'+1)} \qquad 5.38$$

The second integral in equation 5.38 was given in equation 5.35, above. The first integral in equation 5.36 is as follows:

$$\int_{Pr}^{P} V\,dP = [b_{1,i} + b_{2,i}\ T + b_{3,i}\ e^{(-T/300)}].$$

$$(P-Pr) + \frac{b_{4,i}}{2}(P^2-Pr^2) - 35000\ b_{5,i}\ [e^{(-P/35000)} - e^{(-Pr/35000)}]$$

$$5.39$$

In the above equations, $a_{9,i}$ is the constant of integration necessary to satisfy the reference state chosen for the chemical system and replaces the summation of $h_i(Tr)$ and the evaluation of the equations at 298.15 K necessary to satisfy the chosen reference state. In equation 5.38, the last two terms are needed to force continuity in enthalpy because the terms $a_{13,i}$ and $a_{14,i}$ were not constrained to be equal at the critical temperature of the lambda anomaly.

Gibbs Energy of a Phase

Using the reference states given above and the foregoing equations, the Gibbs energy of a phase at temperature and pressure can be calculated from equation 5.40.

$$g_i^\circ = -\frac{a_{1,i}}{6\,T^2} - \frac{a_{2,i}}{2\,T} + a_{3,i}\,(1+\ln T) + 4\,a_{4,i}\,T^{.5}$$

$$+\, a_{5,i}\,(T-T\ln T) - a_{6,i}\,T^2/2 - a_{7,i}\,T^3/6 - a_{8,i}\,T^4/12 + a_{9,i} - a_{10,i}\,T$$

$$+\, g_{M,i}^\circ + \int_{Pr}^{P} V\,dP \qquad 5.40$$

For a phase without a lambda-type anomaly, $g_{M,i}^\circ$ is zero. For a phase with a lambda-type anomaly and at temperatures less than or equal to the critical temperature,

$$g_{M,i}^\circ = a_{13,i} \sum_{k=1}^{n} \frac{T_C\,tau^{j_i'k'+1}}{k'\,(j_i'k'+1)} - \frac{T\,tau^{j_i'k'}}{j_i'\,(k')^2} \qquad 5.41$$

where k' = 2k-1. For a phase with a lambda-type anomaly and at temperatures greater than the critical temperature,

$$g^{\circ}_{M,i} = a_{14,i} \sum_{k=1}^{n} \left\{ \frac{T_C \, tau^{j''_i k'+1}}{k' \, (j''_i k'+1)} - \frac{T \, tau^{j''_i k'}}{j''_i \, (k')^2} \right\}$$

$$+ \; a_{13,i} \sum_{k=1}^{n} \left(\frac{T_C}{k'(j'_i k'+1)} - \frac{T}{j'_i (k')^2} \right) - a_{14,i} \sum_{k=1}^{n} \left(\frac{T_C}{k'(j''_i k'+1)} - \frac{T}{j''_i (k')^2} \right) \qquad 5.42$$

The integral in equation 5.40 was given in equation 5.35, above.

Enthalpy and Gibbs Energy of Formation From the Elements

In the mathematical model developed here, the enthalpy or Gibbs energy for formation of a compound has no special notation. The properties are obtained by writing the chemical equation for the formation of the phase and evaluating the enthalpy or Gibbs energy of reaction in the usual manner as shown by equation 5.43.

$$\Delta_f G^{\circ} = g(\text{phase}) + \sum_{i=1}^{k} n_i \, g(\text{element})_i \qquad 5.43$$

where k is the number of elements in the phase and n_i is the stoichiometric coefficient for each element. The term n_i is negative by convention because the elements are reactants. The difference between this convention and the usual thermodynamic convention is that the elements do not have an assigned value of zero, except, as stated earlier in this chapter, the Gibbs energy of the elements is zero at the reference temperature and pressure, 298.15 K and 1.01325 bar (1 atm), respectively.

Equilibrium Constants and Electrochemical Potentials

The contribution of the ith species to an equilibrium constant or an electrochemical potential was calculated using the equations for the Gibbs energy above, the stoichiometric coefficient n_i, and dividing by "-R T" or "$-n_e$ F", respectively, as indicated in equations 5.07 and 5.08.

Relative Heat Content of a Phase

A commonly measured thermodynamic property is the relative heat content. The relative heat content is the difference in the heat content of a phase or phase assemblage evaluated at two temperatures. The relative heat content or incremental enthalpy data were fit by evaluating h°(T) for the phase stable at the temperature T and h°(Tr) for the phase stable at the reference temperature Tr using equation 5.36. The relative heat content was the difference between the two values. Because the procedure allowed for different phases at T and at Tr, phase inversions provided no obstacle for the evaluation process.

Modelling the Properties of the Wustite Solid Solution

Before one may fit the data for the wustite solid solution and interactions with that complex phase, one must have a model that is useable to describe the nature of the solid solution. In the following sections, the empirical relations and the thermodynamic identities that were used in this study are supplied.

The model used here is the simplest of a large number of possible models that could have been used. However, it will be shown in Chapter 7 that the model is acceptable within the precision of the data.

Empirical Relations Between log $f(O_2)$ and Composition of the Wustite Phase

Empirically, at one atmosphere, log $f(O_2)$ can be considered a linear function of x, the amount of excess oxygen in the wustite formula, FeO_{1+x}. This is equivalent to assuming that the cation vacancies are distributed randomly and that they may be treated as simple point defects. Figure 5.6 shows selected isotherms from several papers. The temperatures range from 965K to 1573K.

Figure 5.6 near here.

$$\log f(O_2) = r(T) + s(T)\,x \qquad 5.44$$

where r(T) and s(T) are functions of the absolute temperature. These can be integrated readily into the functions for the other properties provided that r(T) and s(T) have a form that is compatible with the contribution to the equilibrium constant for the ith phase:

$$
\begin{aligned}
r(T)\ [\text{or } s(T)] = {} & a_{1,r}/(6\ R\ \ln(10)\ T^3) + a_{2,r}/(2\ R\ \ln(10)\ T^2) \\
& - a_{3,r}\ (1 + \ln T)/(R\ \ln(10)\ T) - a_{4,r}\ 4/(R\ \ln(10)\ T^{.5}) \\
& - a_{5,r}\ (1 - \ln T)/R\ \ln(10) + a_{6,r}\ T/(2\ R\ \ln(10)) \\
& + a_{7,r}\ T^2/(6\ R\ \ln(10)) + a_{8,r}\ T^3/(12\ R\ \ln(10)) \\
& - a_{9,r}/(R\ \ln(10)\ T) + a_{10,r}/(R\ \ln(10)) \qquad 5.45
\end{aligned}
$$

The solid lines on Figure 5.6 are calculated isotherms derived from the results of the evaluation given in a later chapter.

Equation 5.45 is the general form if all constants were used. Any prudent evaluator will use only the constants that prove significant. As will be shown in Chapter 7 and in Appendix A, only a few of the constants were used to fit the functions r(T) and s(T).

The Fugacity of Oxygen at the Iron-Wustite and Wustite-Magnetite Boundaries

For thermodynamic calculations, it is useful to have a algebraic expression for the fugacity of oxygen at the wustite boundaries. The utility of these equations will be shown below. Suffice it to say that they eliminated the considerable amount of iteration needed to solve the thermodynamic equations without them.

Equations 5.46 and 5.47 refer to the iron-wustite and the wustite-magnetite boundaries, respectively. As with the fugacity for oxygen in the wustite solid solution field, the function for the fugacity of oxygen, a(T), also was given the form of the contribution to the equilibrium constant given by example for r(T) above.

$$\log f(O_2,iw) = a(T) \qquad 5.46$$

$$\log f(O_2,wm) = b(T) \qquad 5.47$$

In practice, only a few constants were used to fit the data for the fugacity of oxygen, a(T), coexisting with alpha-iron and for the fugacity of oxygen, a'(T), coexisting with gamma-iron. For the wustite magnetite boundary, the function for the fugacity of oxygen, b(T), was also fit using only a few terms.

The Composition of Wustite at the Iron-Wustite and Wustite-Magnetite Boundaries

At equilibrium and for a given temperature T, equation 5.44 and the fugacity of oxygen at the iron-wustite boundary, a(T) [or a'(T)] yield the boundary composition x_a:

$$x_a = \frac{a(T) - r(T)}{s(T)} \qquad 5.48$$

Similarly, the composition x_b at the wustite-magnetite boundary is derived from equation 5.44 and b(T), the fugacity of oxygen at the wustite-magnetite boundary.

$$x_b = \frac{b(T) - r(T)}{s(T)} \qquad 5.49$$

Observations made by Fischer and Hoffmann (1958, 1959), by Hoffmann (1959), and by Touzelin (1974) indicate that wustites of intermediate composition would decompose to nearly stoichiometric FeO and magnetite before finally exsolving to the stable assemblage of iron and magnetite. In this study the compositions of wustite for the metastable extension of the wustite-magnetite boundary were constrained to approach stoichiometric FeO at lower temperatures.

Compositional Width of the Wustite Stability Domain at Constant Temperature and Pressure

Giddings (1972) measured the compositional width of the wustite field by careful coulometric titration. By use of equations 5.48 and 5.49, one may arrive at the following relation:

$$x_b - x_a = \frac{b(T) - a(T)}{s(T)} \qquad 5.50$$

Special Derived Relationships Used in the Data Analysis

The analysis of the data for the Fe-O system allowed several special relations to be used to constrain and reinforce the consistency of the results. Below, constraints on both the properties of the phases as well as the activity of Fe and FeO are developed.

The Activity of Fe in the Wustite Stability Field

For a two-component system, the Gibbs-Duhem relation may be used to derive the activity of one component, provided the activity of the other is known as a function of composition at constant temperature and pressure.

$$N_1 \; \delta \log a_1 \,{}_{T,P} = - N_2 \; \delta \log a_2 \,{}_{T,P} \qquad 5.51$$

where N_1 and N_2 are the mole fractions of each component and a_1 and a_2 are their respective activities. For the binary system Fe-O_2,

$$N(Fe) \; \delta \log a(Fe) = - N(O_2) \; \delta \log a(O_2) \qquad 5.52$$

The activity of O_2(ideal gas) is equal to the fugacity of O_2(ideal gas) divided by the fugacity of the ideal gas at the reference pressure (equation 5.53). Numerically, the activity and the fugacity are equal but the former is unitless while the latter has the unit of bar in the convention followed in this report.

$$\log a(O_2) = \log [f(O_2,bar)/(1\ bar)] \qquad 5.53$$

Given the following chemical formula for wustite, FeO_{1+x},

$$N(Fe) = \frac{2}{(3+x)} \qquad 5.54$$

$$N(O_2) = \frac{(1+x)}{(3+x)} \qquad 5.55$$

From equation 5.44 it can be shown that

$$\delta \log a(O_2) = s(T)\, \delta x \qquad 5.56$$

By systematic substitution of these equations into equation 5.52 and solving, the activity of iron is given by the following equation:

$$\log a(Fe) = \frac{s(T)}{2} x_a + \frac{x_a^2}{2} - x - \frac{x^2}{2} \qquad 5.57$$

where x_a is the amount of excess oxygen in the wustite phase coexisting in equilibrium with metallic iron, as defined by equation 5.48, above.

The Activity of FeO in the Wustite Stability Field

As with the derivation of the activity of Fe as a function of composition at constant temperature and pressure, the activity of FeO in the system $FeO-O_2$ begins with the following equation:

$$N(FeO)\, \delta \log a(FeO) = - N(O_2)\, \delta \log a(O_2) \qquad 5.58$$

Given the formula for wustite, FeO_{1+x},

$$N(FeO) = \frac{2}{(2+x)} \qquad 5.59$$

$$N(O_2) = \frac{x}{(2+x)} \tag{5.60}$$

Using equations 5.58, 5.56, 5.59, and 5.60 above, it can be shown that

$$\log a(FeO) = - \frac{s(T)}{4} x^2 \tag{5.61}$$

Heat Capacity of Wustite Solid Solution

Todd and Bonnickson (1951), among others, measured the heat capacity of a sample of wustite. The sample used for their study had the composition $Fe_{0.947}O$. In discussions in Chapter 7, this composition will be referred to as the "calorimetric composition" or the "calorimetric wustite". This composition has no significance beyond being the sample used for calorimetry. Other compositions were used for measurements but the data are inaccurate and were not used for fitting. All data are discussed in Chapter 7. In the next several paragraphs, the fitting equations for the heat capacity of a wustite of unspecified composition, $Fe_{1-y}O$, are developed. These equations were fit to the data during the optimization.

Consider the following chemical reaction:

$$(1-y)\ FeO + y/2\ O_2 = Fe_{1-y}O \tag{5.62}$$

Then, at equilibrium,

$$\Delta_r G = 0 = \Delta_r G^\circ + (1-y)\ R\ T\ \ln(10)\ \log a(FeO) + y/2\ R\ T\ \ln(10)\ \log a(O_2) \tag{5.63}$$

where

$$\Delta_r G^\circ = g^\circ(\mathrm{Fe}_{1-y}\mathrm{O}) - (1-y)\ g^\circ(\mathrm{FeO}) - y/2\ g^\circ(\mathrm{O}_2) \tag{5.64}$$

By substitution,

$$g^\circ(\mathrm{Fe}_{1-y}\mathrm{O}) = (1-y)\ g^\circ(\mathrm{FeO}) + y/2\ g^\circ(\mathrm{O}_2)$$

$$- (1-y)\ R\ T\ \ln(10)\ \log a(\mathrm{FeO}) - y/2\ R\ T\ \ln(10)\ \log a(\mathrm{O}_2) \tag{5.65}$$

The heat capacity of a phase has the following relation to the Gibbs energy of the phase:

$$C^\circ_{P,i} = - \frac{\delta^2}{\delta T^2}\ g^\circ_i \tag{5.66}$$

Equation 5.66 may be rewritten as follows:

$$C^\circ_p(\mathrm{Fe}_{1-y}\mathrm{O}) = (1-y)\ C^\circ_p(\mathrm{FeO}) + y/2\ C^\circ_p(\mathrm{O}_2)$$

$$+ (1-y)\ \frac{\delta^2}{\delta T^2}\ [R\ T\ \ln(10)]\ \log a(\mathrm{FeO})] + y/2\ \frac{\delta^2}{\delta T^2}\ [R\ T\ \ln(10)]\ \log a(\mathrm{O}_2)] \tag{5.67}$$

In the calorimetric measurements, $C^\circ_p(\mathrm{Fe}_{1-y}\mathrm{O})$ was observed. The fitted functions for FeO, log a(FeO), and log $a(\mathrm{O}_2)$ must be consistent with these data. Of course, these same fitted functions must also be consistent with the other experimental data accepted as valid for the optimization.

Entropy of the Wustite Solid Solution

Beginning with the same reaction as for heat capacity above, and using the relation

$$S_i^\circ = -\frac{\delta}{\delta T} g_i^\circ \tag{5.68}$$

one may readily show that the entropy of a wustite of composition $Fe_{1-y}O$ can be defined as the following equation.

$$\begin{aligned} S^\circ(Fe_{1-y}O) &= (1-y)\ S^\circ(FeO) + y/2\ S^\circ(O_2) \\ &+ (1-y) \frac{\delta}{\delta T} [R\ T\ \ln(10)]\ \log a(FeO)] + y/2 \frac{\delta}{\delta T} [R\ T\ \ln(10)]\ \log a(O_2)] \end{aligned} \tag{5.69}$$

Equation 5.69 was used in the optimization as the fitting function for the entropy of $Fe_{1-y}O$.

Heat Content of the Wustite Solid Solution

The heat content or incremental enthalpy for wustite was calculated using the following relation:

$$h^\circ(Fe_{1-y}O) = g^\circ(Fe_{1-y}O) + T\ S^\circ(Fe_{1-y}O) \tag{5.70}$$

The Gibbs energy, $g^\circ(Fe_{1-y}O)$, and the entropy, $S^\circ(Fe_{1-y}O)$, are defined in equations 5.65 and 5.68, respectively. The heat content for wustite was calculated by evaluating equation 5.70 at T and at Tr and then calculating the difference:

$$[H°(T)-H°(Tr)](Fe_{1-y}O) = h°(Fe_{1-y}O,T) - h°(Fe_{1-y}O,Tr) \qquad 5.71$$

Reactions Including Wustite as a Component

Much of the data for reactions that included wustite were reported either as values of log $a(O_2)$, log $[P(CO_2)/P(CO)]$, log $[P(H_2O)/P(H_2)]$ or potential differences relative to another buffer reaction or to oxygen gas at some fixed pressure. (At the relatively low pressures, one atmosphere or less, it was assumed that the gases behaved ideally and the pressures of the gas, divided by the reference pressure, could be replaced by the activity of the gas, a_i.) For example, Ackermann and Sanford (1966) reported log $[P(CO_2)/P(CO)]$ values for various compositions of wustite within the stability field. The chemical reaction was as follows:

$$FeO(wus,sln) + CO(g) = Fe(wus,sln) + CO_2(g) \qquad 5.72$$

The equilibrium constant for this reaction is given by equation 5.73.

$$\log K = \log a(Fe) + \log a(CO_2) - \log a(FeO) - \log a(CO) \qquad 5.73$$

Solving for log $[a(CO_2)/a(CO)]$, one obtains equation 5.74.

$$\log [a(CO_2)/a(CO)] = \log K - \log a(Fe) + \log a(FeO) \qquad 5.74$$

For equation 5.72, at equilibrium,

$$\log K = \frac{-1}{R\ T\ \ln(10)} [g°(Fe) + g°(CO_2) - g°(FeO) - g°(CO)] \qquad 5.75$$

From equation 5.57,

$$\log a(Fe) = \frac{s(T)}{2} x_a + \frac{x_a^2}{2} - x - \frac{x^2}{2} \qquad 5.76$$

The term x_a is defined by equation 5.48 in the preceding section.

From equation 5.61,

$$\log a(FeO) = - \frac{s(T)}{4} x^2 \qquad 5.77$$

Then, for a given x in the formula FeO_{1+x},

$$\log [a(CO_2)/a(CO)] = \frac{-1}{R\ T\ \ln(10)} [g°(Fe) + g°(CO_2) - g°(FeO) - g°(CO)]$$

$$- \frac{s(T)}{2} x_a + \frac{x_a^2}{2} - x - \frac{x^2}{2}$$

$$- \frac{s(T)}{4} x^2 \qquad 5.78$$

During the fitting procedure, Ackerman and Sanford's (1966) data and all similar data were fit by such an equation. For log $a(O_2)$ or log

$[a(H_2O)/a(H_2)]$ data and for electrochemical potentials relative to another buffer assemblage or to a fixed activity of oxygen gas, adjustments were made in equation 5.72. In fitting, equations similar to 5.78 were used for those data sets.

Data reported for the iron-wustite boundary were treated in the same way except that log a(Fe) was defined as zero and x was defined as x_a (equation 5.48).

For the wustite-magnetite boundary, the reaction used was either

$$Fe_3O_4\text{(magnetite)} + CO(g) = 3\ FeO(s) + CO_2(g) \qquad 5.79$$

or

$$0.25\ Fe_3O_4\text{(magnetite)} + CO(g) = 0.75\ Fe(s) + CO_2(g) \qquad 5.80$$

In these cases, x was defined as x_b as in equation 5.49, above. The fitting equations were, respectively,

$$\log [a(CO_2)/a(CO)] = \frac{-1}{R\ T\ \ln(10)} [3\ g°(FeO) + g°(CO_2) - g°(Fe_3O_4) - g°(CO)]$$

$$+ 3 \frac{s(T)}{4} x_b^2 \qquad 5.81$$

or

$$\log [a(CO_2)/a(CO)] = \frac{-1}{R\ T\ \ln(10)} [0.75\ g°(Fe) + g°(CO_2) - 0.25\ g°(Fe_3O_4) - g°(CO)]$$

$$- 0.25 \frac{s(T)}{2} x_a + \frac{x_a^2}{2} - x_b - \frac{x_b^2}{2} \qquad 5.82$$

In summary, all reactions that included wustite were treated in the same way. The chemical reaction was defined in terms of FeO as a component and adjustments were made in terms of x, the amount of excess oxygen in the formula.

Temperature of the Breakdown of Wustite to Iron and Magnetite

At the breakdown temperature, that is at the isobaric invariant point where the phases iron, magnetite, wustite, and vapor coexist, the following functions must be coincident:

$$\log f(O_2,iw) = a(T) \qquad 5.83$$

$$\log f(O_2,wm) = b(T) \qquad 5.84$$

$$\log f(O_2) = 0.5 \log K[Fe_3O_4 = 3\ Fe + 2\ O_2] \qquad 5.85$$

$$\log f(O_2) = \log a(FeO,\ iw) - \log K[2\ FeO = 2\ Fe + O_2] \qquad 5.86$$

$$\log f(O_2) = - \log a(FeO,\ wm) - \log K[2\ Fe_3O_4 = 6\ FeO + O_2] \qquad 5.87$$

The first two equations are empirical representations of the log $f(O_2)$ - temperature dependence of the iron-wustite and the wustite-magnetite equilibria. (See also equations 5.46 and 5.47 above.) The last three functions are the log $f(O_2)$ - temperature dependencies as calculated from the equilibrium constants indicated by the reaction in the brackets. In equation 5.85, the phases iron and magnetite are stoichiometric and at unit activity. No activity corrections were necessary. However, for equations 5.86 and 5.87, corrections for the decreased activity of FeO at the iron-wustite and at the wustite-magnetite boundary were necessary.

Without the addition of some other constraints, it would be fortuitous if the available experimental data as analysed using the mathematical model would give the required coincidence in temperature and composition of the wustite solid solution at a fixed pressure. Let us analyse the available data for strength and weakness in order to choose some observation that can be fixed safely and not cause undue distortion in the fitting.

(1) Composition of the solid solution at the triple point. In the course of assembling the data, critical reading of the source manuscripts showed that all data on the composition of the wustite solid solutions are derived from indirect observations. There are no direct measurements available for guiding a logical choice of the composition coexisting with iron and magnetite.

(2) Thermodynamic data and experimental studies on the oxidation of iron to magnetite below the isobaric invariant point. The combustion and solution calorimetry are not of sufficient accuracy to fix the fugacity of oxygen at the isobaric invariant point. The errors are generally in excess of 1300 J/mol for the formation of magnetite from the elements and leads to an error of about 0.08 in the log $f(O_2)$. Addition of errors

from the inaccuracies in entropy and heat capacity would increase this error to greater than 0.10. The H_2O/H_2 ratios coexisting with magnetite and iron below the isobaric invariant point are also inaccurate. Refer to Figures. A.32 through A.37 in Appendix A.

(3) The breakdown temperature of wustite at 1 bar. The following temperatures are reported for the isobaric equilibrium among the phases iron, wustite, magnetite, and vapor.

Temperature		Data Source
570°C	843.15 K	Chaudron (1921)
565°C	838.15 K	Eastman (1922)
570°C	843.15 K	Eastman and Evans (1924)
560°C	833.15 K	Schenck and Dingmann (1927)
559°C	832.15 K	Emmett and Shultz (1933)
569°C	842.15 K	Barbi (1964a)
572°C	845.15 K	Barbi (1964a)
577°C	850.15 K	Barbi (1964a)
569°C	842.15 K	Barbi (1964b)
565°C	838.15 K	Birks (1966)
570°C	843.15 K	Rau (1972)
554°C	827.15 K	Barbero and others (1981)

A least-squares fitting of the weighted data for the iron-wustite and the wustite-magnetite boundaries, yielded a temperature of 839.15 K (or 566°C). This temperature was used as the isobaric invariant point at one atmosphere because it is also in agreement with the list of observations given above. By using the "polymorph" feature of the optimization routine (Haas, 1974), the fugacities of oxygen at the iron-wustite and wustite-magnetite boundaries, a(T) and b(T), respectively, were forced to be identical at 839.15 K.

Summary

The general thermodynamic relations, the empirical functions for V°, C_p°, and log $a(O_2)$, and the derived relations for log a(Fe), log a(FeO), $C_p^\circ(Fe_{1-y}O)$, $S^\circ(Fe_{1-y}O)$, $H^\circ(T)-H^\circ(Tr)$ for $Fe_{1-y}O$, and reactions including wustite are given above.

The philosophy used during the course of this optimization was to develop a fitted model that was consistent with all that was known for the chemical systems. If an observation could be calculated from one or more of the equations in the model, the observation and the associated precision was included in the data set that was to be fitted. As will be demonstrated in Chapter 7, this effort paid dividends in detecting erroneous experimental data and in exposing misconceived ideas.

CHAPTER 6

DATA EVALUATED

All types of data indicated by equations in the preceding chapter were contained in the fitted data set. In summary a total of over 8,000 observations and theoretical constraints were used in the optimization. Every attempt was made to use the primary observations such as gas ratios, heat capacities, electrochemical potentials, and so forth, if available, in preference to calculated log $a(O_2)$ data or values derived from equations.

Instead of publishing the experimental data, many authors chose to publish equations only. Where the equations described chemical reactions, the observed property (Gibbs energy difference, equilibrium constant, or electrochemical potential) were calculated at appropriate intervals, such as every 50 kelvin within the range of the study, and these calculated values were entered into the data set. In this study, no use was made of an author's fitted slopes and intercepts.

Most, but not all, of the observations and the calculated values are shown graphically and in summary tables in the next chapter where the results are discussed. The remainder are discussed in Appendix A.

CHAPTER 7

RESULTS AND DISCUSSION OF THE EVALUATION

Introduction

It is worth restating again that the optimization presented here was the result of a "simultaneous" fitting of all functions given in Chapter 5 to the data for the chemical system. Because all functions and constraints were fit in one operation, the resulting properties for each phase and for the interactions among the phases did not depend upon a few observations but was the result of evaluating the entire data set taken collectively. Because many observations and many constraints were used in this optimization, minor changes, such as adding or deleting some data sets or some constraints, would have little significance in the final results. The evaluated data sets contained redundant data. The changes that would have the most significant effect on the evaluation would be changes in one or more of the empirical equations given in Chapter 5, above. Justification for the empirical equations used in this report is that they do describe the available data adequately from 200 to 1800 K and up to pressures in excess of 100 kb.

To avoid chaos, the discussion will follow approximately the order in which the equations and thermodynamic properties are given in Chapter 5. The discussion will start with molar volumes and related data, then continue with thermal data, entropy, enthalpies of formation, compositional data for the wustite stability field, and conclude this chapter with activities of Fe and

FeO. All reaction equilibria are given in Appendix A.

Molar Volume

Copper and the Oxides of Copper

A survey of the volumetric data for copper and the oxides of copper was not made at this time. It was left for future research.

Nickel, Ni(s,l)

The survey of the volumetric data for nickel was superficial. The data contained in citations in the compilation by Clark (1966) were augmented by the expansivities of the solid reported by Fraser and Hallett (1961) and by Nix and MacNair (1941) and the densities of the liquid reported by Saito and others (1969a,b). The following equations were the results of the least-squares fitting of the data. Figures 7.01 through 7.03 show the fitted curve and the experimental data. Refer to Table 7.01. For the solid metal,

$$V(\mathrm{cm}^3/\mathrm{mol}) = [6.4165 + 0.35902\cdot10^{-3}\ T + 0.008750\ e^{(-T/300)}] \cdot[1. - 0.50260\cdot10^{-6}\ P] \qquad 7.01$$

For the liquid,

$$V(\mathrm{cm}^3/\mathrm{mol}) = 5.6645 + 1.0232\cdot10^{-3}\ T \qquad 7.02$$

Figures 7.01 through 7.02 and Table 7.01 near here.

Bunsenite, NiO(s)

The monoxide of nickel has a lambda-type Neèl transition at 519 K. Above this temperature, bunsenite is paramagnetic. The crystal structure is the cubic halite structure. Below 519 K, bunsenite is antiferromagnetic and has a rhombohedral structure that is progressively more distorted along the [111] direction of the high-temperature cubic phase as temperature decreases below 519 K. The rhombohedral crystallographic modification was ignored in fitting the lower temperature data. This lack of accuracy was minor. Figures 7.04 and 7.05 show the correlation between the fitted Equation 7.03 and the data cited on Table 7.02.

$$V(\mathrm{cm^3/mol}) = [10.6575 + 0.50147\cdot10^{-3}\,T + 0.008496\,e^{(-T/300)}]$$
$$\cdot[1. - 0.34255\cdot10^{-6}\,P + 13.653\cdot10^{-3}\,e^{(-P/35000)}] \qquad 7.03$$

As with nickel, there is a lack of fit in the vicinity of the Neel temperature. But, more importantly, the high-temperature data measured by Leipold and Niel~~s~~sen (1964) were not used in the optimization. The data, if correctly measured, indicate an anomalous increase in the coefficient of volumetric expansion. There is no justification for such an expansion.

Figures 7.04 through 7.05 and Table 7.02 near here.

Iron, Fe(alpha=bcc=s1, beta=fcc=s2)

Metallic iron is a body-centered close-packed cubic structure (bcc) and is ferromagnetic below the Curie temperature of 1042 K. The ferromagnetic to paramagnetic transition does have an expression in the molar volumes but the structure does not change. At 1184 K, the face-centered close-packed cubic structure (fcc) becomes stable at one bar total pressure and persists to 1665 K where iron reverts to the alpha or bcc structure. The melting point is 1809 K.

The data for alpha- and gamma-iron (Table 7.03) were fit with equations 7.04 and 7.05, respectively. For alpha-iron,

$$V(\mathrm{cm}^3/\mathrm{mol}) = [6.77756 + 0.38690\cdot 10^{-3}\ T + 0.12143\ e^{(-T/300)}] \cdot [1. - 0.33286\cdot 10^{-6}\ P + 21.7861\cdot 10^{-3}\ e^{(-P/35000)}] \qquad 7.04$$

For gamma-iron,

$$V(\mathrm{cm}^3/\mathrm{mol}) = [6.4797 + 0.5177\cdot 10^{-3}\ T + 0.3623\ e^{(-T/300)}] \cdot [1. - 0.30110\cdot 10^{-6}\ P + 27.831\cdot 10^{-3}\ e^{(-P/35000)}] \qquad 7.05$$

Figures 7.06 through 7.08 show the results. Again, near the lambda-type anomaly, the function contains a minor inaccuracy in fitting the data for the alpha phase. For most thermochemical applications, this has no significance.

The experimental data of Esser and Muller (1933) shown on Figure 7.06, part b, has the same expansivity as the other isobaric studies, but the absolute data reported in the study are systematically off by 0.02 cm^3/mol. This may have been an equipment or calibration error.

Figures 7.06 through 7.07 and Table 7.03 near here.

Ferrous Oxide, FeO, and the Wustite Solid Solution, $Fe_{1-y}O$

The data for the wustite solid solution are summarized on Table 7.04. Hentschel (1970) and more recently Simmons (1980) have shown that the cubic cell edge of quenched wustite at room temperature is a linear function of the amount of iron deficit from the stoichiometric formula, FeO.

$$a_0 = c_0 + c_1(1-y) \qquad 7.06$$

The available data at room temperature and one bar are compared with the fitted curve on Figure 7.09. Equation 7.07 was used to calculate the fitted curve.

$$\begin{aligned} V(\mathrm{cm}^3/\mathrm{mol}) = {} & [11.8563 + 0.617125\cdot10^{-3}\ T + 369.056\ e^{(-T/300)}] \\ & \cdot[1. - 0.53957\cdot10^{-6}\ P + 4.5581\cdot10^{-3}\ e^{(-P/35000)}] \\ & - 23.5379\ y + 2.270\ y^2 - 0.07298\ y^3 \qquad 7.07 \end{aligned}$$

The experimental data of Touzelin (1974) between 1073 and 1348 K and the fitted curves are show on Figure 7.10. Based on these data and the fit of the data, the linearity in a_0 at elevated temperature is also valid. Other data measured at high temperatures were scattered and were not necessarily measured under controlled oxygen potentials. It must be noted that the study by Hayakawa and others (1972) is not consistent with the oxygen activities calculated from their reported CO_2-CO gas mixtures. The data were given zero weight.

Figure 7.11 shows the effect of pressure on the wustite structure. The correlation is based on the experimental measurements of Hazen (1981). The other data at elevated pressure were less consistent. The study by Clendennen and Drickamer (1966) is anomalous and was given zero weight in the fitting.

Whereas a calibration curve between composition and X-ray-determined cell edges might work for temperature-quenched wustites*, such a curve must be used with caution for pressure-quenched samples. Hazen and others (1981) note that wustites do not show ideal elastic behavior when held at pressures in excess of 150 kb for periods of weeks. For example, a sample held at 170 kb for 14 days, then at 200 kb for an additional 14 days was 0.8 percent smaller than before the pressure treatment. This was discussed in detail by Jeanloz and Hazen (1983). The reason for this behavior is unknown but may be due to diffusion-controlled ordering of defects at elevated pressures.

Like bunsenite, wustite has a Neél transition from antiferromagnetic to paramagnetic behavior at about 190 K. Also like bunsenite, this tranistion is first order. The cubic <u>halite</u> structure which exists at temperatures above 190 K becomes progressively distorted along the [111] cubic direction to a rhombohedral structure with decreasing temperature. The effect of pressure on the Neel temperature is given by equation 7.08 (Zou and others 1980) where pressure is expressed in bars.

$$T_N(K) = 190. + 0.002163\ (P-1) \qquad 7.08$$

Table 7.05 gives the measured Neel temperatures as a function of composition. The data are conflicting. For this reason, a Neél temperature

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* A prudent experimentalist would construct a calibration curve from data that the experimentalist observed in that laboratory. The cell edge a_0 will vary with the quench procedure used in a laboratory.

temperature of 190 K was used in this study and no compositional variation was allowed.

Figures 7.09 through 7.11 and Tables 7.04 and 7.05 near here.

Hematite, $Fe_2O_3(s)$

Hematite is an antiferromagnetic solid with the corundum structure which exists at room temperature and one bar. Between 248 and 265 K and one bar pressure, hematite undergoes a second-order Morin transition. This transition has been studied by Umebayashi and others (1966), Searle (1967), and by Worlton and Decker (1968). Up to approximately 6 kb this transition has a slope of 0.0037±0.0002 K/b. Above this pressure, the slope is considerably less. At 298 K, the transition is between 20 and 30 kb. The ranges in these data are due to hyster~~y~~esis in the measurements. There is a slight but detectable change in the compressibility of hematite near 30 kb (Sato and Akimoto, 1979) but this has been ignored in this evaluation.

Hematite has a Neél transition at 955.5 K and one bar. This transition has a negative slope (Mao and others, 1977) and is located between 550 and 630 kb at 298 K. Assuming a linear dependence,

$$T_N(K) = 955.53 - 0.00112(\pm 0.00007)\cdot(P - 1) \qquad 7.09$$

Table 7.06 shows the experimental data used to derive equation 7.10, below. Figures 7.12 and 7.13 show the correlation between the fitted equation and the data.

$$V(cm^3/mol) = [29.7593 + 1.30076\cdot 10^{-3}\,T + 0.48106\,e^{(-T/300)}]$$

$$\cdot[1. - 0.46005\cdot 10^{-6}\,P - 1.6415\cdot 10^{-3}\,e^{(-P/35000)}] \qquad 7.10$$

Figures 7.12 through 7.13 and Table 7.06 near here.

Fayalite and the Diferrous Silicate Liquid, $Fe_2SiO_4(sl,l)$

The volumetric properties of fayalite are given on Figures 7.14 through 7.16. The solid lines on these Figures were calculated from the fitted equations below. For fayalite,

$$V(\text{cm}^3/\text{mol}) = [44.8974 + 1.66293\cdot10^{-3}\,T + 0.442294\,e^{(-T/300)}] \cdot[1. - 0.49420\cdot10^{-6}\,P + 13.4370\cdot10^{-3}\,e^{(-P/35000)}] \tag{7.11}$$

For the diferrous silicate ~~liqid~~ liquid, $V(\text{cm}^3/\text{mol}) = 50.0395\cdot[1. + 8.00758\cdot10^{-3}\,e^{(-P/35000)}]$

Table 7.07 has a summary of the available data. The volume of the liquid diferrous silicate was derived from the melting curves for fayalite and the spinel phase and the thermal functions for all three phases. The enthalpy of melting of fayalite at one bar was taken from the analysis by Stebbins and Carmichael (1984). These data will be discussed in a section on reactions below.

Figures 7.14 through 7.16 and Table 7.07 near here.

Diferrous Silicate (Spinel Structure), $Fe_2SiO_4(s2)$

Table 7.08 cites the available volumetric data for the high-pressure dimorph of fayalite. The phase has a normal spinel structure. The magnetic transition is below 100 K. Figure 7.17 and 7.18 show the available experimental data and the fitted curves calculated from equation 7.13.

$$V(\mathrm{cm}^3/\mathrm{mol}) = [42.0021 + 2.8523\cdot 10^{-4}\,T - 1.01528\,e^{(-T/300)}] \cdot [1. - 0.35156\cdot 10^{-6}\,P + 8.7455\cdot 10^{-3}\,e^{(-P/35000)}] \qquad 7.13$$

Within the precision of the measurements, the effect of pressure as measured by Mao and others (1969), Sato (1977), and Wilburn and Bassett (1978) are equivalent. At one bar, however, the volume measured by Marumo and others (1977) is too large by about 1.33 cm^3/mol. The phase equilibria indicate the smaller value of 42.076±0.049 cm^3/mol is preferred. This is close to the measured values of 42.03±0.02 cm^3/mol reported by Mao and others (1969) and of 42.076±0.014 cm^3/mol reported by Yamanaka (1986). The data measured by Yamanaka (1986) at 873 and 973 K are too large and would indicate an anomaly in the coefficient of volume expansion. These data were given zero weight.

Figures 7.17 through 7.18 and Table 7.08 near here.

Magnetite, $Fe_3O_4(s)$

Magnetite is a cubic, inverse spinel above the Verwey transition that is located at approximately 110 to 125 K and has a negative slope. For geological applications, the properties of this low-temperature phase is of no importance. Magnetite changes from a ferrimagnetic solid to a paramagnetic solid at the Neèl temperature of 849.1 K. The effect of pressure on the critical temperature, T_N is shown on Figure 7.19 and was fit by equation 7.14 where P is in bars.

$$T_N(K) = 849.1 + 0.002002_9 \cdot (P - 1) \qquad 7.14$$

The molar volume of magnetite is given by equation 7.15 where pressure is in bars and temperature is in kelvins.

$$V(cm^3/mol) = [42.9347 + 2.73147 \cdot 10^{-3}\, T + 1.26153\, e^{(-T/300)}]$$
$$\cdot [1. - 0.386024 \cdot 10^{-6}\, P + 7.37298 \cdot 10^{3}\, e^{(-P/35000)}] \qquad 7.15$$

The experimental data are cited on Table 7.09 and both the data and the fitted curves are given on Figures 7.20 through 7.21.

Gorton and others (1965) clearly show the effect of magnetic disordering on the molar volume. The fitted equation does not contain terms for fitting the anomaly and some inaccuracy does result. Sharma's (1950) data were given zero weight because the data do not indicate the existance of any magnetic anomaly but should have.

Mao and others (1974) observed a first order transition in magnetite at about 250 kb at room temperature and tentatively identified the high-pressure phase as monoclinic. Huang (1987) reinvestigated the inversion. At room temperature, the reversal bracket spans from 250 kb with increasing pressure to less than 50 kb with decreasing pressure. At 873 K (600°C), the bracket is about 50 kb wide and centers on about 110 kb. Based on Huang's interpretation of his data, the inversion lies near 200 kb at 298 K but could vary from about 145 to 255 kb. The slope of the pressure-temperature inversion curve is -0.0081 K/bar but, conceivably, could vary from -0.0207 to -0.00045 K/bar. No attempt was made in this compilation to evaluate the thermodynamic properties of the high-pressure "monoclinic" phase.

Carel and Vallet (1981) proposed a first-order change in magnetite at 1433 K and ambient pressure. This is discussed in the next section on heat capacity.

Figures 7.19 through 7.21 and Table 7.09 near here.

Molar Heat Capacity and Heat Content Data

Introduction

All available data above 200 K were evaluated. Some data between 100 and 200 K were also included where it was useful to get better definition of the low-temperature curvature or of the function around Neèl transitions.
In general, data below 200 K were not used because the empirical equations are not applicable as temperature approaches 0 K and because data in this range of temperatures have little application in the earth sciences. Data that exist for temperatures below 200 K were generally not cited in the tables in this section.

On the tables, the error is given as x.x±y.y percent.
The x.x represents the average error of the fitted curve from the experimental data and the y.y represents the average deviation of the error about the average error. For example, +1.2±0.4 percent indicates that
the data average 1.2 percent larger than the fitted curve and the 0.4 represents the average scatter of the errors about the 1.2 percent value. Or stated differently, the average experimental value lies between 0.8 and 1.6 percent higher than the fitted curve.

Tenorite, CuO(s)

The experimental data for the heat capacity and relative heat content (incremental enthalpies) are cited on Table 7.10 and are plotted on Figures 7.22 and 7.23. The insert on Figure 7.22 shows the data measured by Hu and Johnson (1953) and the calculated curve near the Neèl temperature, 227 K. The data by Clusius and Harteck (1928) and by Millar (1929) were given zero weight. For tenorite,

$$\begin{aligned} C_P^\circ\ [\mathrm{J/(mol\ K)}] = {} & 1.42819\cdot10^{6}\ T^{-2} \\ & - 4.20905\cdot10^{4}\ T^{-1} \\ & + 3.28723\cdot10^{3}\ T^{-0.5} \\ & - 30.1998 \\ & + 2.20428\cdot10^{-2}\ T \\ & + C_M^\circ \end{aligned} \tag{7.16}$$

where, for $T = 227$ K ($\leq T_N$),

$$C_M^\circ\ [\mathrm{J/(mol\ K)}] = 2.19256 \sum_{k=1}^{7} \frac{\tau^{(2k-1)}}{(2k-1)} \tag{7.17}$$

and where, for $T > 227$ K,

$$C_M^\circ\ [\mathrm{J/(mol\ K)}] = 1.92047 \sum_{k=1}^{7} \frac{\tau^{-5(2k-1)}}{(2k-1)} \tag{7.18}$$

Figures 7.22 through 7.23 and Table 7.10 near here.

Cuprite and the Dicuprous Oxide Liquid, $Cu_2O(s,l)$

The data for cuprite are cited on Table 7.11. The data of Hu and Johnson (1951) were not used because they were not consistent with the high-temperature data of Mah and others (1967) and because the entropy calculated from these data (Gregor, 1962) was too large to be in agreement with the phase equilibria.

Figures 7.24 and 7.25 show plots of the experimental data and the fitted equations, 7.19 and 7.20. The enthalpy of melting of Cu_2O is 65,653 J/mol at 1516.7 K. For cuprite,

$$\begin{aligned} C_p^\circ\ [\mathrm{J/(mol\ K)}] = {} & 1.25417\cdot10^6\ T^{-2} \\ & - 3.53957\cdot10^4\ T^{-1} \\ & + 2.73479\cdot10^3\ T^{-0.5} \\ & + 2.92731\cdot10^{-2}\ T \end{aligned} \qquad 7.19$$

For the liquid Cu_2O,

$$C_p^\circ\ [\mathrm{J/(mol\ K)}] = 99.6136 \qquad 7.20$$

Figures 7.24 through 7.25 and Table 7.11 near here.

Bunsenite, NiO(s)

The experimental data for bunsenite are cited on Table 7.12 and plotted on Figure 7.26 and 7.27. Equation 7.21 is a fit of these data.

The experimental data of King and Christensen (1958) are too low by about 2 percent. The measurements by Hemingway (1984) and by Tomlinson and others (1955) are in good agreement except the highest value measured by Tomlinson and others. This value is 2 percent too small and was given zero weight in the optimization. The data of King and Christensen (1958) were the only data available for the temperatures above 1108 K. In order to fit this region the data were not used directly. Instead, the differences in heat contents between adjacent observations were calculated and fit. The weights used were the same as the absolute magnitude of the precision for the original data.

The experimental data measured by Lewis and Saunders (1973) between 325 and 650 K and by Mainard (1963) between 300 and 575 K were not available for inclusion in the evaluation. The data were presented as a smooth graph only and errors in scaling the heat capacity from the graphs would exceed two percent. Had the tables of data been available, Hemingway (1984) would not have had to repeat the measurements.

$$
\begin{aligned}
C^\circ_p\ [\mathrm{J/(mol\ K)}] = {} & 4.20397\cdot 10^6\ T^{-2} \\
& - 9.43725\cdot 10^4\ T^{-1} \\
& + 7.13873\cdot 10^3\ T^{-0.5} \\
& - 110.6966 \\
& + 3.1427\cdot 10^{-2}\ T \\
& + C^\circ_M \qquad\qquad 7.21
\end{aligned}
$$

where, for $T \leq 519$ K ($= T_N$),

$$C_M^\circ\ [\mathrm{J/(mol\ K)}] = 8.50694 \sum_{k=1}^{7} \frac{\tau^{3(2k-1)}}{(2k-1)} \qquad 7.22$$

and where, for T > 519 K,

$$C_M^\circ\ [\mathrm{J/(mol\ K)}] = 8.10930 \sum_{k=1}^{7} \frac{\tau^{-15(2k-1)}}{(2k-1)} \qquad 7.23$$

The lambda anomaly at 519 K represents an approximately 4.0-J/(mol K) increase in entropy and a 1,730-J/mol increase in enthalpy.

Figures 7.26 through 7.27 and Table 7.12 near here.

Ferrous Oxide, FeO, and Wustite, $Fe_{1-y}O$ or FeO_{1+x}

The available experimental data for wustite are cited on Table 7.13 and are plotted on Figures 7.28 through 7.30. The curves were calculated from equation 7.24, below.

$$C_p^\circ(\text{wustite}) = 1\text{-}y\ C_p^\circ(\text{FeO}) + \frac{y}{2}\,C_p^\circ(O_2) + T\,\frac{d^2}{dT^2}\left[(1-y)\,R\,T\,\ln a(\text{FeO}) + \frac{y}{2}\,R\,T\,\ln a(O_2)\right] \qquad 7.24$$

Refer to Chapter 5 for the derivation of this equation. The heat capacity of FeO was calculated from the fitted equation below.

$$\begin{aligned} C_p^\circ\ [\text{J/(mol K)}] = {} & 5.68242\cdot10^{7}\ T^{-3} \\ & - 9.71854\cdot10^{5}\ T^{-2} \\ & - 1.69293\cdot10^{3}\ T^{-1} \\ & + 4.37416\cdot10^{2}\ T^{-0.5} \\ & + 33.7527 \\ & + 9.72807\cdot10^{-3}\ T \\ & + C_M^\circ \end{aligned} \qquad 7.25$$

where, for $T \leq 190$ K ($= T_N$),

$$C_M^\circ\ [\text{J/(mol K)}] = 11.07758 \sum_{k=1}^{7} \frac{\tau^{3(2k-1)}}{(2k-1)} \qquad 7.26$$

and where, for $T > 190$ K,

$$C_M^\circ\ [\text{J/(mol K)}] = 8.31625 \sum_{k=1}^{7} \frac{\tau^{-15(2k-1)}}{(2k-1)} \qquad 7.27$$

In fitting equation 7.24 to the data, the temperature of the lambda anomaly, T_N, was kept constant with composition at 190 K. Koch and Fine (1967), Michel and others (1970) and Mainard and others (1968) studied the variation of T_N with composition and published conflicting results as were given on Table 7.05.

Mainard and others (1968) measured the heat capacities for five wustite samples from "1-y" = 0.899 to "1-y" = 0.944 moles. Unfortunately, they only supplied a graph of $C_p/(C_p \text{ at } T_N)$ for each composition and gave no data that would enable the calculation of absolute heat capacities. Qualitatively, the fitted curve is in agreement with the data of Mainard and others (1968) though the Neél temperatures differed and the ratios for temperatures above T_N are somewhat larger than are indicated by the work of Todd and Bonnickson (1951). This is another example of poor judgement of what should be published. Unfortunately, to get the absolute heat capacities the research will have to be repeated because the experimental data are not available.

Rogez and others (1982) measured the heat content between 1179 and 299 K for samples of wustite varying from y = 0.0562 to y = 0.1166 moles. (Refer to Figure 7.30.) The data were nearly 5 percent low when compared with the work of Coughlin and others (1951). An attempt to adjust the data measured by Coughlin and others (1951) downward by about 5 percent to agree with Rogez and other's (1982) study produced unacceptable distortions in the fitting of the equilibria. Coughlin and others' (1951) data were accepted as correct. It should be noted that the trend of the fitted curve parallels the data measured by Rogez and others (1982).

The lambda anomaly represents an approximately 5.1-J/(mol K) increase in entropy and an approximately 790 J/mol increase in enthalpy.

Figures 7.28 through 7.30 and Table 7.13 near here.

Hematite, $Fe_2O_3(s)$.

A summary of the data used to fit the model are given in Table 7.14. The studies by Esser and others (1933), by Roth and Bertram (1929), by Parks and Kelley (1926), and by Reznitsky and Filippova (1972) were given zero weight. The work used poorly described samples. Because better data were available, these data were not needed. As for magnetite and bunsenite, the heat contents of Coughlin (1951) were recalculated and entered in the file of fitted data as differences in heat content between adjacent experimental temperatures. The precision used as a guide in fitting was the absolute magnitude of the precision for the original measurements.

Figures 7.31 and 7.32 show the experimental data and the fitted curves as calculated by the following equation.

$$\begin{aligned} C^\circ_P\ [\mathrm{J/(mol\ K)}] = {} & 3.73378 \cdot 10^{6}\ T^{-2} \\ & - 9.71352 \cdot 10^{4}\ T^{-1} \\ & + 6.54451 \cdot 10^{3}\ T^{-0.5} \\ & + 2.77769 \cdot 10^{-02}\ T \\ & + C^\circ_M \end{aligned} \qquad 7.28$$

where, for T = 955.53 K (= T_N),

$$C^\circ_M\ [\mathrm{J/(mol\ K)}] = 25.7486 \sum_{k=1}^{7} \frac{\tau^{3(2k-1)}}{(2k-1)} \qquad 7.29$$

and where, for T > 955.53 K,

$$C^\circ_M\ [\mathrm{J/(mol\ K)}] = 17.6061 \sum_{k=1}^{7} \frac{\tau^{-15(2k-1)}}{(2k-1)} \qquad 7.30$$

The lambda anomaly associated with the Neél temperature represents an approximately 11.7-J/(mol K) increase in entropy and about 9,100-J/mol increase in the enthalpy of hematite. Reactions in which hematite is a phase should exhibit significant curvature between 900 and 960 K as a result of this second-order transition.

Figures 7.31 through 7.32 and Table 7.14 near here.

Fayalite and the Diferrous Silicate Liquid, Fe_2SiO_4(sl,l)

Table 7.15 cites the sources of data used to refine the heat capacity and heat content of fayalite and Fe_2SiO_4(l) as shown on Figures 7.33 and 7.34.

Osako's (1980) data are clearly in error and were not used. Roth and Bertram (1929) measured the heat content of a natural sample of unknown composition. These data were also given zero weight. The results are given by the lines on the graphs and by equations 7.31 and 7.32.

For fayalite, Fe_2SiO_4(sl),

$$\begin{aligned} C_p^\circ\ [\mathrm{J/(mol\ K)}] = {} & 1.99298\cdot 10^{6}\ T^{-2} \\ & - 3.77927\cdot 10^{4}\ T^{-1} \\ & + 3.10914\cdot 10^{2}\ T^{-0.5} \\ & + 220.7439 \\ & - 8.03640\cdot 10^{-3}\ T \end{aligned} \qquad 7.31$$

For the diferrous silicate liquid, Fe_2SiO_4(l),

$$C_p^\circ\ [\mathrm{J/(mol\ K)}] = 226.833 \qquad 7.32$$

Stebbins and Carmichael (1984) determined that the heat of fusion of fayalite as measured by Orr (1953) was in error. Iron would exsolve from the melt and alloy into the Pt-10Rh capsule. The composition would migrate away from iron towards $Fe_3O_4\cdot 2SiO_2$ that is the reported composition of the mineral laihunite. The hypothetical congruent heat of fusion of fayalite at 1490 K of 89.3 kJ/mol as determined by Stebbins and Carmichael (1984) and phase equilibria were used to correct the drop calorimetry and to determine the heat content of the liquid.

Figures 7.3 through 7.34 and Table 7.15 near here.

Diferrous Silicate (spinel structure), $Fe_2SiO_4(s2)$

Measurements have become available since 1980 on the heat capacity of the spinel dimorph of fayalite. These data are cited on Table 7.16 and plotted on Figures 7.35 and 7.36. The measurments of Osako (1980) are discordant and were given zero weight. The fitted curve (Equation 7.33) represents the best estimate based on the data and on the available phase equilibria for the three polymorphs, fayalite, the spinel structure, and the liquid.

$$\begin{aligned} C_p^\circ[J/(mol\ K)] = &- 4.41874\cdot 10^{5}\ T^{-2} \\ &- 1.72553\cdot 10^{3}\ T^{-0.5} \\ &+ 236.469 \\ &+ 1.38599\cdot 10^{-3} \end{aligned} \qquad 7.33$$

Figures 7.35 through 7.36 and Table 7.16 near here.

Magnetite, $Fe_3O_4(s)$

The experimental data used to evaluate the heat capacity of magnetite are cited on Table 7.17 and plotted on Figures 7.37 and 7.38. The older studies (those made before 1950) were made using natural magnetites of unknown composition. These studies were given zero weight. Experimental heat capacities in the studies listed below were published as graphs only and could not be included in this evaluation. Because of discrepancies among the research of Bartel and Westrum (1975), Coughlin and others (1951), and of Gronvold and Sveen (1974), it is indeed unfortunate that the authors did not make the data available in tabular form.

SOURCE	TEMPERATURE RANGE
Dixon and others (1965)	1.2 to 4.7 K
Gmelin and others (1983)	5 to 130 K
Gmelin and others (1984)	80 to 125 K
Matsui and others (1977)	77 to 160 K
Rigo and others (1983)	4 to 17 K, 77 to 180 K
Shepherd and others (1985)	5 to 350 K
Sukharevskii and others (1970)	12 to 160 K
Todo and Chikazumi (1977)	7 to 50 K

The data of Gronvold and Sveen (1974) are systematically higher than the data of Bartel and Westrum (1975). However, the data in both sets were given equal weight. The departure of the fitted equation from the heat capacities measured by Gronvold and Sveen (1974) near 1000 K was due in part to an anomalous and unexplained inflection in the measurements, in part to the low values required by the the relative heat content data of Coughlin and others

(1951), especially at temperatures above 1000 K, and in part to the available phase equilibria.

As with bunsenite and hematite, the heat content data were the only information in addition to the reaction equilibria that would constrain the fitted constants at temperatures above 1000 K. Above the anomaly at 849 K, the heat content data were not used directly. Instead, the differences in the heat contents between adjacent experimental temperatures were calculated and fit by the mathematical model. The precisions used for each point were the absolute precisions for the original data. Equation 7.34 is the result of the optimization.

$$\begin{aligned} C_P^\circ\ [\mathrm{J/(mol\ K)}] = &-1.12425\cdot10^{9}\ T^{-3} \\ &+ 2.51675\cdot10^{7}\ T^{-2} \\ &- 3.31526\cdot10^{5}\ T^{-1} \\ &+ 2.11896\cdot10^{4}\ T^{-0.5} \\ &- 225.613 \\ &+ 6.48354\cdot10^{-2}\ T \\ &+ C_M^\circ \end{aligned} \qquad 7.34$$

where, for T = 849.1 K (= T_N),

$$C_M^\circ\ [\mathrm{J/(mol\ K)}] = 63.8383 \sum_{k=1}^{7} \frac{\tau^{4(2k-1)}}{(2k-1)} \qquad 7.35$$

and where, for T > 849.1 K,

$$C_M^\circ\ [\mathrm{J/(mol\ K)}] = 47.5655 \sum_{k=1}^{7} \frac{\tau^{-15(2k-1)}}{(2k-1)} \qquad 7.36$$

The lambda anomaly at 849 K represents an approximately 22.9-J/(mol K) increase in entropy and an approximately 16,800-J/mol increase in enthalpy. Reactions where magnetite is a reacting phase should exhibit significant curvature between 800 and 865 K as a result of this second-order anomaly.

Carel and Vallet (1981) proposed an endothermic first-order change in magnetite at 1433 K. The standard change in enthalpy was reported as -9,990 J/mol when heating. This could not be confirmed to exist either by crystallography, calorimetry, nor thermochemistry and was not allowed in this study.

Figures 7.37 through 7.38 and Table 7.17 near here.

Entropy

Table 7.18 gives the reported data for S°(T)-S°(0) as derived from integration of calorimetric data and the entropies, S°(T), derived from the optimization of the data. The fitted entropies are consistent with the experimental S°(T)-S°(0) and with the various reactions to be discussed in the following section except as follows.

The entropy of King (1957) for bunsenite was clearly too high when the heat capacity data measured by Hemingway (1984), the combustion calorimetry of Boyle and others (1954), and the reaction data (For example, refer to Figures A.15 or A.30 in Appendix A.) were considered. The accepted value is 1.29 J/(mol K) lower than the value reported by King (1957). Such corrections are consistent with errors caused by overestimation of the entropy change between 0 K and the lowest temperatures achieved in the earlier calorimeters used in the studies at the U.S. Bureau of Mines (R.A. Robie, 1987, personal communication).

Todd and Bonnickson (1951) proposed a 1.71-J/(mol K) contribution to the entropy of the calorimetric sample for wustite, $Fe_{0.947}O$. This would allow for the disorder of the defects. Humphrey and others (1952), Chase and others (1985), and this study found support for an entropy near 57.49 J/(mol K). In part, crystallographic evidence supports ordering of defects at 298 K and in part, there is both magnetic ordering and a first-order crystallographic inversion near 190 K. Residual disorder at 0 K may not exist. However, because there is the possibility that the extrapolation to 0 K from 54 K by Todd and Bonnickson (1951) may have overestimated the entropy contribution in that temperature region, at this writing, it is not certain that a disorder contribution sould be included. The only certainty is that the thermochemical data support the entropy at 298.15 K of 57.61 J/(mol K) as found in this study. Sorting this out has been left to future research.

The entropy of magnetite found in this study was lower than that found by integration by Westrum and Gronvold (1969). The optimized value is 0.71 J/(mol K) lower and is more in line with the thermochemical data at high temperatures and with the somewhat lower heat capacities measured by Bartel and Westrum (1975) and heat contents measured by Coughlin and others (1951). There are arguments for a residual entropy for magnetite where S°(0) ranges from 3.38 to 11.51 J/(mol K) (Westrum and Gronvold (1969). This was not supported by this study. To this author, the mobility of charge in magnetite, coupled with the magnetic ordering and the first-order crystallographic changes that occur at the Verwey transition near 110 to 124 K would produce an ordered structure as the temperature approached 0 K.

Table 7.18 near here.

Enthalpy, Gibbs Energy and Related Properties

Introduction

Various aspects of a chemical reaction are measured experimentally as changes in enthalpy, changes in Gibbs energy, equilibrium constants or electrochemical potentials. The data are measures of the properties of a group of phases. The properties of specific phases conform to these observations. For each stoichiometric compound, there exists an unique heat capacity, entropy, enthalpy, and volume that is a function of temperature and pressure. For a solid solution, such as wustite, $Fe_{1-y}O$, composition is an additional variable. The task of an evaluator is to find the right description that will permit calculation of the properties of the phases and of the interactions among the phases that are in agreement with the available experimental data. In the preceding sections, descriptions of the properties of specific phases were given. In this section, the results will be given where those descriptions are combined to calculate the properties of the group of phases. In Appendix A, the results for each study will be given by reaction. Studies that were accepted or rejected will be discussed in the appendix.

Scope of Reactions Considered

In order to supply an understanding of the scope of this study, the chemical network evaluated in this study is shown schematically on Figure 7.39. In addition to the solids containing Cu, Ni, and Fe, the gases H_2(g), H_2O(g), CO(g), and CO_2(g) are shown. Thermodynamic properties for these elements and gases, for O_2(g), and for SiO_2(quartz, cristobalite) were taken from other research as discussed in Chapter 3. The straight lines connecting the labeled symbols represent reactions 3.01 through 3.09 plus reactions 7.37 and 7.38.

$$CO(g) + 0.5\ O_2(g) = CO_2(g) \tag{7.37}$$

$$H_2(g) + 0.5\ O_2(g) = H_2O(g) \tag{7.38}$$

Reaction 3.01 is represented as a straight line between the labels Cu and Cu_2O. The curved lines, then, represent the cross reactions where the oxygen is balanced out of the chemical reactions represented by the straight lines. For example, the curved line connecting the pair Cu and Cu_2O with the pair Ni and NiO represents reaction 39.

$$2\ Cu(s) + NiO(bunsenite) = Cu_2O(cuprite) + Ni(s) \tag{7.39}$$

Experimental data were available for all reactions represented by straight lines connecting the Cu-, Ni-, and Fe-bearing lables, and for all reactions represented by curves.

In Appendix A, the reactions will be discussed by beginning with the copper oxides, then nickel oxide, then the iron oxides and finally the iron silicates.

Figure 7.39 near here.

Third-Law Calculations of $\Delta_r H°$ at 298.15 K

Following the approach outlined by Stull and Prophet (1971), the enthalpy of reaction for each observation was calculated and plotted as a function of the temperature of observation. These plots proved useful in identifying inconsistent experimental data. They will be supplied in the appendix with the discussion of each reaction. The appropriate equations for calculating $\Delta_r H°(298)$ from Gibbs energy data, equilibrium constants, and electrochemical potentials are given below.

$$\Delta_r H°(298) = \Delta_r G°(T) - T\,\Delta gef°(T) \qquad 7.40$$

$$\Delta_r H°(298) = -[R\,T\,\ln K°(T) + T\,\Delta gef°(T)] \qquad 7.41$$

$$\Delta_r H°(298) = -[n_e\,F\,E°(T) + T\,\Delta gef°(T)] \qquad 7.42$$

where

$$\Delta gef°(T) = \sum_{i=1}^{j} n_i \cdot gef_i°(T) \qquad 7.43$$

and $$gef_i°(T) = \frac{g_i°(T) - h_i°(298)}{T} \qquad 7.44$$

In equation 7.42, n_e is the number of electrons exchanged in the chemical reaction. In equation 7.43, the term n_i is the stoichiometric coefficient of the *i*th phase in the chemical reaction, and by convention, is positive for products and negative for reactants.

Tenorite, CuO(s)

Table 7.19 summarizes the results for reactions containing tenorite, the cupric oxide. Column 2 gives the results of the weighted, least-squares optimization. Column 3 gives the average enthalpy of reaction for each reaction. The enthalpy of formation (last column) was calculated from column 3. In this calculation, the properties of the other phases were assumed to be correct. This has the effect of indicating what the maximum deviations would be. The last entry at the bottom of the table gives the results from this study. The use of weighting accounts for the averages from the reactions being slightly more negative than the recommended enthalpy of formation of -155.660±0.209 kJ/mol.

Table 7.19 near here.

Cuprite, $Cu_2O(s)$

The results for cuprite are summarized on Table 7.20. The string "-----" indicates that all data for the reaction were given zero weight. Therefore, there was no average enthalpy of reaction for those reactions. The different columns have the same meaning as given under tenorite, above. The recommended enthalpy of formation is -170.631±0.226 kJ/mol. This compares favorably with the averages that vary from -170.390 to -170.905 kJ/mol.

Table 7.20 near here.

Bunsenite, NiO(s)

Table 7.21 contains the summary of the data for bunsenite. The recommended enthalpy of formation is -240.277±0.374 kJ/mol. The averages for the eight reactions vary from -239.939 to -240.762 kJ/mol. These are within acceptable limits. Only the most negative enthalpy is found outside the 2-sigma value. The agreement in enthalpies as show on Table 7.21 was only possible by adjusting the entropy of bunsenite downward as shown on Table 7.18.

Table 7.21 near here.

Ferrous Oxide, FeO(s)

The results for ferrous oxide are given on Table 7.22. Again, the columns have the same meaning as for tenorite, above. In calculating the enthalpies of reaction, the data were first corrected to the stoichiometric composition FeO by using the activities of O_2, Fe, and FeO as necessary.

The recommended enthalpy of formation is -262.133±0.923 kJ/mol*. This compares favorably with the averages that vary from -262.558 to -261.843 kJ/mol. The first of the two entries for the reaction "$2\ FeO = 2\ Fe + O_2$" is the average derived from log $a(O_2)$-x data for the solid solution. Refer to Table A.10 in Appendix A. The second entry is for data given for the iron-wustite equilibrium. Refer to Table A.11 in Appendix A.

The agreement among the various reactions, temperatures, and compositions is an indication that the solid solution model as described in Chapter 5 and fitted to the data in this study is acceptable within the limits of the data. For example, refer to Figures 7.40 through 7.43. These are third-law enthalpy-temperature plots and third-law enthalpy-composition plots for all data within the wustite solid solution field that were used in the optimization. The chemical reactions are given below. For Figures 7.40 and 7.41,

$$FeO(wus,sln) + CO(g) = Fe(wus,sln) + CO_2(g) \quad . \qquad 7.45$$

---

* This error includes the error in the calculation of log a(FeO) and log $a(O_2)$ of 0.031 at 839.15 K. Without the adjustment, the error would be 0.411 kJ/mol for the enthalpy of formation.

$$FeO(wus,sln) + H_2(g) = Fe(wus,sln) + H_2O(g) \qquad 7.46$$

The modifier "(wus,sln)" indicates the component is in solution in the wustite solid solution phase.

Using equation 7.45 as an example, one can readily derive $\Delta_r H°(298)$ using the third-law relations, the activities of Fe and FeO, and the Gibbs energy functions.

$$\begin{aligned}\Delta_r H°(298) = &- R\ T\ \ln(10)\ \log\ [a(CO_2)/a(CO)]\\ &- R\ T\ \ln(10)[2\ \log\ a(Fe) - 2\ \log\ a(FeO)]\\ &- T\ [2\ gef°(Fe) + gef°(O_2) - 2\ gef°(FeO)] \qquad 7.47\end{aligned}$$

The Figures, then, are the third-law enthalpies calculated using the experimental gas ratios plotted as a function of temperature and of composition. There is no anomalous trend either with temperature or composition except for the data supplied by Marion (1955). The 14 values at temperature greater than 1250 K indicate disequilibrium probably caused by Soret phenomenon. Refer to Appendix A, page A16, for further discussion. In Appendix A, third-law plots as a function of composition are supplied for all solution data by source.

One must note that the results are model-dependent. A condition for use in other calculations is that the model be acceptable and not in violation with any assumptions made in those calculations. If a user does not follow this restriction, inconsistencies and additional inaccuracies will develop in the calculations.

Figure 7.40 through 7.43 and Table 7.22 near here.

Hematite, $Fe_2O_3(s)$

Table 7.23 gives the results for hematite. The recommended enthalpy of formation of hematite from the elements is -824.928±3.158 kJ/mol~~§~~-1. This is in good agreement with the averages that vary from -824.991 to -824.539 kJ/mol. The most aberrant average, -824.539 kJ/mol, was measured under difficult conditions of low temperatures and with varying H_2O-H_2 ratios. The lack of agreement for this reaction should be expected.

Table 7.23 near here.

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§ The error includes 3.000 kJ/mol added because of the uncertain~~s~~ty in magnetite. Without the addition, the error would be 0.149 kJ/mol for hematite which is clearly too small.

Fayalite, the Spinel Dimorph and the Diferrous Silicate liquid, Fe_2SiO_4(s1,s2,l)

Tables 7.24 and 7.25 show the data for fayalite and the spinel dimorph that is stable at high pressures. The stability fields are shown graphically on Figure 7.44. Refer to the discussion of the polymorphic reactions in Appendix A for details.

Of the phases evaluated, the data for fayalite and its dimorph are least consistent. The recommended enthalpy for formation of fayalite is -1477.733 ±1.324 kJ/mol. This is consistent with the averages that vary from -1477.706 to -1474.380 kJ/mol. The enthalpy of inversion of the spinel phase to fayalite at 298.15 K and one bar is -6.767±3.064 kJ/mol. The metastable enthalpy of melting of fayalite at 1490 K and one bar is 88.05±2.32 kJ/mol. The metastable enthalpy of melting of the spinel dimorph at 1090 K and one bar is 70.3±4.1 kJ/mol.

For fayalite, much of the scatter in the data is caused by the sluggish nature of the silicate reactions, both at one bar and at higher pressures. For the spinel dimorph, the scatter is also due to sluggish reactions. At elevated pressure, the reversals in the phase equilibria are generally in excess of 3 kilobars apart at constant temperature.

Figure 7.44 and Table 7.24 and 7.25 near here.

Magnetite, $Fe_3O_4(s)$

Table 7.26 contains the summary of the reactions in which magnetite was a phase. The recommended enthalpy of formation of magnetite from the elements at 298.15 K and one bar is -1116.640±2.245 kJ/mol†.

The averages for the tabulated reactions vary from -1118.860 to -1115.830 kJ/mol. Most are near the recommended value. The most divergent values given on Table 7.26 are for reactions where fayalite was also a phase. The other divergent value, -1118.370 kJ/mol, is for the reaction "$3\ Fe + 2\ O_2 = Fe_3O_4$" which may be observed directly only below 839.15 K. At those low temperatures, slowness to equilibrate make the observations difficult.

One of the major contributions to fixing the properties of magnetite is the coexistance of iron, wustite, and magnetite at 839.15±10 K.

This equilibrium temperature, which is effectively a fixed point because of the narrow temperature range, constrains the iron-magnetite equilibrium. Even though there is some scatter in the data used to derive the thermal functions, this produces minor variation by comparison.

Table 7.26 near here.

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† The error has been adjusted to include the error for calculation of "3 log a(FeO) + 0.5 log $a(O_2)$" at 839.15 K which is 0.125. Without the adjustment, the error would have been 0.235 for the formation of magnetite at 298.15 K.

Special Relations

The Activity of O_2 Within the Wustite Stability Field

The activity of O_2 within the wustite stability field was discussed in Appendix A, pages A.??ff., in detail. The activity as a function of x may be calculated from equations 7.48, 7.49, and 7.50. Figure 7.45 shows the activity-of O_2 as a function of temperature and composition. Table 9.15 through 9.18 give log $a(O_2)$ and the related functions

$\overline{S}(O_2)-\overline{S}°(O_2)$,

$\overline{H}(O_2)-\overline{H}°(O_2)$,

and $\overline{G}(O_2)-\overline{G}°(O_2)$

from x = 0.0 to 0.16 moles from 800 to 1700 K.

$$\log f(O_2) = r(T) + s(T)\, x \tag{7.48}$$

$$r(T) = 5.36060\,(1 + \ln T) - 0.71074\cdot 10^{-3}\, T - (3.57076\cdot 10^{4})/T + 45.9213 \tag{7.49}$$

$$s(T) = 4.39866\cdot 10^{-3}\, T + 17.3524 \tag{7.50}$$

Figure 7.45 near here.

The Activity of O_2 at the Iron-Wustite Field Boundary

The activity of O_2 at the iron-wustite field boundary would normally be calculated from the equilibrium constant (equation 7.52) for the reaction between iron and wustite (equation 7.51) and the activity of O_2 within the wustite field (equation 7.48).

$$2\ \mathrm{FeO(wus,sln)} = 2\ \mathrm{Fe(s)} + O_2(g) \tag{7.51}$$

where

$$\log a(O_2,\mathrm{wus,sln}) = \log K + 2 \log a(\mathrm{FeO}) \tag{7.52}$$

However, to obtain the solution, one must iterate to determine the composition at which equations 7.48 and 7.52 are equal. To avoid the costly iteration, equation 7.53 and 7.54 were fit and used to calculate $\log a(O_2)$ at the field boundary coexisting with alpha-Fe and gamma-Fe, respectively. Table 10.4 gives $\log a(O_2,\mathrm{iw})$ from 800 to 1700 K.

$$\begin{aligned}\log a(02,\mathrm{iw}) = a(T) = {} & 1.27402\cdot 10^{3}\ T^{-0.5} \\ & - 14.85341\ [1-\ln(T)] \\ & - 2.266454\cdot 10^{-3}\ T \\ & - 3.502370\cdot 10^{4}\ T^{-1} \\ & - 111.5396\end{aligned} \tag{7.53}$$

$$\begin{aligned}\log a(02,\mathrm{iw}') = a'(T) = {} & 8.919244\cdot 10^{-1}\ [1-\ln(T)] \\ & - 2.877354\cdot 10^{4}\ T^{-1} \\ & + 13.20823\end{aligned} \tag{7.54}$$

The Activity of O_2 at the Wustite-Magnetite Field Boundary

As for the iron-wustite field boundary, the normal approach is to solve for the composition of the boundary using equations 7.48, 7.55, and 7.56.

$$2\ Fe_3O_4(\text{magnetite}) = 6\ FeO(\text{wus,sln}) + O_2(g) \qquad 7.55$$

where

$$\log a(O_2,\text{wus,sln}) = \log K - 6 \log a(FeO) \qquad 7.56$$

To avoid costly iteration, equation 7.57 was fit and used to calculate the activity of $O_2(g)$ at the wustite-magnetite field boundary. Table 10.7 gives log $a(O_2,\text{wm})$ from 800 to 1700 K.

$$\begin{aligned}\log a(O_2,\text{wm}) = b(T) = & -1.098206\cdot10^6\ T^{-2} \\ & - 4.702740\cdot10^2\ T^{-0.5} \\ & + 97.50838\ [1-\ln(T)] \\ & + 1.979987\cdot10^{-2}\ T \\ & + 1.084638\cdot10^4\ T^{-1} \\ & + 764.6720 \end{aligned} \qquad 7.57$$

The Activity of Fe Within the Wustite Stability Field

The activities of Fe(alpha) between 800 and 1184 K and above 1665 K and of Fe(gamma) between 1184 and 1665 K were calculated at 0.1 intervals in y from y = 0 to 0.16 using equation 5.57. The data are shown on Figure 7.46. The lines crossing the contours represent the iron-wustite and the wustite-magnetite boundaries (upper, horizontal line and lower line with negative slope, respectively). Table 9.11 through 9.14 give log a(Fe) and the related functions

$\overline{S}(Fe)-\overline{S}°(Fe)$

$\overline{H}(Fe)-\overline{H}°(Fe)$

and $\overline{G}(Fe)-\overline{G}°(Fe)$

from x = 0.0 to 0.16 moles from 800 to 1700 K.

There are no direct measurements of the activity of Fe in the wustite solid solution to which the calulated values may be compared.

Figure 7.46 near here.

The Activity of FeO Within the Wustite Stability Field

The activity of FeO between 800 and 1700 at 0.1 intervals in y from y = 0 to 0.16 were calculated from equation 5.61. These are plotted on Figure 7.47. The lines crossing the contours represent the iron-wustite and the wustite-magnetite boundaries (upper line and lower line with negative slope, respectively). Table 9.19 through 9.22 give log a(FeO) and the related functions

$\overline{S}(FeO)-\overline{S}^\circ(FeO)$

$\overline{H}(FeO)-\overline{H}^\circ(FeO)$

and $\overline{G}(FeO)-\overline{G}^\circ(FeO)$

from x = 0.0 to 0.16 moles from 800 to 1700 K.

There are no direct measurements of the activity of FeO in the wustite solid solution to which the calulated values may be compared.

Figure 7.47 near here.

Boundary Compositions for the Wustite Stability Field

The Iron-Wustite Boundary

As indicated previously, direct observations of the composition of the wustite stability boundaries do not exist. The available compositions were gained by comparing two sets of measurements each with a different condition kept constant. For example, Ackermann and Sanford (1966) varied the ratio of the CO_2 and CO gases at constant temperature and noted the composition of wustite. These data were compared with the CO_2-CO ratio that gave the two phase iron-wustite equilibrium as a function of temperature.

The mathematical model used in the optimization had to conform within the precision of the data to the derived values. For the iron-wustite equilibrium, the compositions in equilibrium with alpha- and gamma-iron are, respectively,

$$x_a = \frac{a(T) - r(T)}{s(T)} \qquad 7.58$$

and

$$x_{a'} = \frac{a'(T) - r(T)}{s(T)} \qquad 7.59$$

Figure 7.48 shows the available data for the iron-wustite boundary. The lines, in addition to the iron-wustite boundary, are supplied to keep the figure in context with the balance of the wustite stability field. Agreement is reasonable considering the quality of the data. The electrochemically derived data are the most discordant. In the electrochemical cells, control of the composition was difficult. The mass of wustite was small. Oxygen gas diffuses slowly through the electrolyte into or out from the chamber containing only wustite. This gain or loss of oxygen makes it difficult to control composition. This is best shown on Figure 7.49. Ariya and Yakovleva (1970) measured potentials between wustites of constant composition and the iron-wustite boundary and between the wustite-magnetite boundary and the iron-wustite boundary. Their data for the wustite-magnetite boundary are in good agreement with the results of other studies and with the results of this optimization. However, their reported potentials for the wustite-only experiments are consistent with a wustite that contains less oxygen than the compositions that they state. The data show that oxygen diffused away from the solid solution sample to the reference buffer iron+wustite where it would convert the iron to more wustite.

The major departure from the data for the iron-wustite boundary is the composition of wustite at the iron-wustite-magnetite isobaric equilibrium. This will be taken up at the end of this section.

Note must be given to the agreement with the metastable iron-wustite equilibrium observed by Touzelin (1974) and by Hoffmann (1959). Refer to Figures 48, parts b and c. The dashed line and the arrow on the figures are the metastable extensions of the iron-wustite equilibrium. Experimental attempts to follow the iron-wustite equilibrium to lower temperatures (to greater metastability) always encountered magnetite nucleation and complete decomposition of the wustite.

Figure 7.48 and 7.49 near here.

The Wustite-Magnetite Boundary

As with the iron-wustite equilibrium, all fitted values were derived indirectly from experimental data. Figure 7.50 gives the derived values and the position of the fitted boundary (Equation 7.60).

$$x_b = \frac{b(T) - r(T)}{s(T)} \tag{7.60}$$

The lines, in addition to the wustite-magnetite boundary, are supplied to keep the figure in context with the balance of the wustite stability field. Agreement with electrochemically derived values and with some gas equilibria at high excess oxygen concentrations is poor. The observation by Darken and Gurry (1945) at 1673 K indicates an excess oxygen content too large to be in agreement with the log $a(O_2)$-temperature data for the wustite-magnetite boundary, b(T). The values derived by Engell (1957), Vallet and Raccah (1965), Lykasov and others (1969), and Touzelin (1974) are in good agreement.

The metastable observations by Fischer and Hoffmann (1958, 1959) were not fit below 800 K, though the calculated boundary does approach x = 0 at 298 K. Hentschel (1970) observed that x = 0 at 498 K whereas the calculated value is near 0.036 moles excess oxygen. Accuracy should not be expected because the data are too few and too poorly observed to be fit properly. Also, no allowance was made in fitting the empirical function b(T) for the heat effect associated with the Neel transition of magnetite. The magnetic ordering with decreasing temperature increases the stability of magnetite. The heat effect should sharply reduce the metastable wustite stability field below 850 K as indicated by the observations of Fischer and Hoffmann (1958, 1959).

Refinement of the model at lower temperatures must await (1) additional data on the heat capacity of wustites with higher excess oxygen than are presently available, (2) evaluation of data for ternary "wustite" containing other elements such as the magnesiowustite, (Mg,Fe)O, and (3) more attention given to both composition and oxygen potentials of wustites at higher pressure where the stability field extends to lower temperatures and to more iron-rich compositions.

Figure 7.50 near here.

Width of the Wustite Stability Field

Sockel and Schmalzried (1968) and Giddings (1972) measured the compositional width of the wustite stability field. Their data and the fitted equation, 7.61 are plotted on Figure 7.51. Agreement is good.

$$x_b - x_{a'} = \frac{b(T) - a'(T)}{s(T)} \qquad 7.61$$

Figure 7.51 near here.

The Composition of Wustite at 839.15 K

A much ignored point made by Darken and Gurry (1945, 1946) was the nature of the method they used to define the boundary compositions below 1373 K (1100°C). Though they clearly stated that the supplied values below 1373 K were estimates, the estimates were accepted as "facts". Giddings (1972) arrived at very similar compositions but he also used the same assumptions for the extrapolation. Spencer and Kubachewski (1978) and E~~i~~sdale (1983) accepted Darken and Gurry's results without change. Knacke (1983) built on the evaluation by Giddings (1972). The phase diagram and the thermodynamic data supplied by the latter authors all closely followed Darken and Gurry's (1945, 1946) original di~~i~~agram and results.

Even this author accepted the estimated composition of wustite at the iron-wustite-magnetite equilibrium until it became apparent during the course of the evaluation that these "facts" were not in agreement with the experimental data for the chemical system. At that time it because apparent that the fitted functions were in agreement with the troublesome data reported by Fischer and Hoffmann (1958, 1959), Hoffmann (1959), Herai and Manec (1964), Hentschel (1970), and Touzelin (1974).

Fischer and Hoffmann (1958, 1959), and Hoffmann (1959) observed that the composition obtained upon decomposition of wustite at 550°C (823 K) was independent of the composition of the starting wustite and on the temperature of synthesis. The compositions were near $Fe_{0.92}O$. Such compositions would not be expected from the short metastable extensions of the boundary curves on the phase diagram supplied by Darken and Gurry (1945) (Figure 3.4). However, the compositions are consistent with the result of this evaluation as shown on Figures 7.48 and 7.50. In addition, the continued extension of the iron-wustite boundary curve is consistent with the wustite coexisting with iron reported by Touzelin at 713 K (Figure 7.48). Also, it is in qualitative agreement with the wustites coexisting with magnetite between 523 and 753 K as reported by Fischer and Hoffmann (1958, 1959) as shown on Figure 7.50.

Summary

In the foregoing sections of this chapter, it was shown that one can develop a set of thermodynamic data for the chemical systems through careful reading and analysis of the published literature and through careful least-squares fitting of those data believed to be correctly reported. The next three chapters contain the following data calculated from that model:

(1) thermodynamic tables for the oxides and for fayalite along with tables of data for the reference elements and compounds used in this study,

(2) tables of properties for the wustite solid solution that are consistent with the tables for the other phases,

and (3) tables of standard electrochemical potentials and fugacities of oxygen coexisting with the solid chemical buffers for oxygen.

Appendix B gives the constants for use in the equations that were developed in Chapter 5 and used in this chapter.

CHAPTER 8

RECOMMENDED TABLES OF THERMODYNAMIC PROPERTIES

The following tables of thermodynamic properties were calculated from the least-squares fitting of the mathematical model given in Chapter 5 to the cited data. The 2-sigma confidence limits for C_p°, S°, V°, H(T)-H(Tr), and the Gibbs energy function were calculated at 298.15 K (= Tr) and at every 250-K isotherm using the variance-covariance matrix developed from the least-squares fitting. For details of the calculation of the confidence limits, refer to Appendix C or to Clifford (1973).

For $\Delta_f H^\circ$, $\Delta_f G^\circ$, and $\log_f K^\circ$, the confidence limit could not be evaluated completely. The functions used for the elements, and for the oxides of carbon, hydrogen, and silicon were derived from smoothed tables and not from the original experimental data. For the properties describing the formation of a compound from the elements, the confidence limit was increased to 4 sigma. Any additional variance that might have arisen from fitting the experimental data for the auxiliary phases should lie well within the 4-sigma limit for fitting the oxides evaluated here. This is consistent with the author's experience in fitting the thermal functions for nickel, iron, quartz, and cristobalite.

The tables are arranged alphabetically by chemical formula as listed below. For convenience, the tables for the auxiliary phases are also given with the same alphabetical sequence.

Table Number	Mineral Name	Formula
8.01	Graphite	$C(s)$
8.02	---	$CO(g)$
8.03	---	$CO_2(g)$
8.04	Copper	$Cu(s,l)$
8.05	Tenorite	$CuO(s)$
8.06	Cuprite	$Cu_2O(s,l)$
8.07	Iron	$Fe(s1,s2)$
8.08	---	$FeO(s)$
See Ch. 9	Wustite	$Fe_{1-y}O$
8.09	Hematite	$Fe_2O_3(s)$
8.10	Fayalite	$Fe_2SiO_4(s1,l)$
8.11	---	$Fe_2SiO_4(s2)$
8.12	Magnetite	$Fe_3O_4(s)$
8.13	---	$H_2(g)$
8.14	Ice, water, ---	$H_2O(s,l,g)$
8.15	---	$H_2O(g)$
8.16	Nickel	$Ni(s)$
8.17	Bunsenite	$NiO(s)$
8.18	---	$O_2(g)$
8.19	---	$Si(s)$
8.20	Cristobalite	$SiO_2(s)$
8.21	Quartz	$SiO_2(s)$

Table 8.01 through 8.21 near here.

CHAPTER 9

PROPERTIES OF THE WUSTITE SOLID SOLUTION

Introduction

The tables in this chapter supply the thermodynamic properties of the wustite solid solution. The tables were calculated using the appropriate functions in Chapter 5 and the fitted constants derived from the optimization. For most tables, no special significance was attached to the composition of the calorimetric sample, $Fe_{0.947}O$ ($y = 0.053$). However, to accomodate those who are addicted to using that composition for calculations, the data are given on Tables 9.23 through 9.26.

It must be noted that the calorimetric sample is metastable below 1075 K. Between 1075 and 839 K, alpha-iron and a wustite having a higher excess oxygen content is stable. Below 839 K, alpha-iron and magnetite are stable.

Extrapolation in Composition and Temperature

All properties were derived from the apparent linear relation between log $a(O_2)$ and x, the moles of excess oxygen in the wustite formula, FeO_{1+x}. The functions are valid between the iron-wustite boundary and the wustite-magnetite boundary between 839 K and 1700 K. Extrapolations to compositions outside of the stability range are based on the extension of the linear relation between log $a(O_2)$ and x to lower or higher values of x. To the extent that the linearity is valid as x becomes smaller or larger, so also the data for the metastable wustite are valid.

Extrapolations to lower temperatures are based

(1) on the fitting of the heat capacity, entropy, and heat content data for the calorimetric sample,

(2) on the approximation that wustite coexisting with magnetite becomes stoichiometric at lower temperatures,

and (3) on reasonable extensions of the functions r(T) and s(T). Modelling the heat capacity of wustite as a function of the heat capacity for "FeO" and the heat capacity for Fe_3O_4 less the magnetic contribution C°_M for magnetite produced very similar results at low temperatures. The model was not used because the model was not internally consistent and because the differences were not significant.

Data Tables

The tables in this chapter are as follows:

Table	Title
9.01	Composition of wustite at the iron-wustite boundary and the activities of Fe, FeO, and O_2 between 800 and 1700 K at one bar total pressure.
9.02	Composition of wustite at the wustite-magnetite boundary and the activities of Fe, FeO, and O_2 between 800 and 1700 K at one bar total pressure.
9.03	Molar volume of wustite for $y = 0$ to $y = 0.16$ between 200 and 1700 K at one bar total pressure.
9.04	Molar heat capacity of wustite for $y = 0$ to $y = 0.16$ between 200 and 1700 K at one bar total pressure.
9.05	Molar entropy of wustite for $y = 0$ to $y = 0.16$ between 200 and 1700 K at one bar total pressure.
9.06	Molar heat content of wustite for $y = 0$ to $y = 0.16$ between 200 and 1700 K at one bar total pressure.
9.07	Molar Gibbs energy function of wustite for $y = 0$ to $y = 0.16$ between 200 and 1700 K at one bar total pressure.
9.08	Entropy change for formation of wustite for $y = 0$ to $y = 0.16$ between 800 and 1700 K at one bar total pressure.
9.09	Enthalpy change for formation of wustite for $y = 0$ to $y = 0.16$ between 800 and 1700 K at one bar total pressure.
9.10	Gibbs energy change for formation of wustite for $y = 0$ to $y = 0.16$ between 800 and 1700 K at one bar total pressure.
9.11	The function $\overline{S}(Fe)-\overline{S}^\circ(Fe)$ in wustite for $y = 0$ to $y = 0.16$ between 800 and 1700 K at one bar total

pressure.

9.12 The function $\overline{H}(Fe)-\overline{H}^\circ(Fe)$ in wustite for y = 0 to y = 0.16 between 800 and 1700 K at one bar total pressure.

9.13 The function $\overline{G}(Fe)-\overline{G}^\circ(Fe)$ in wustite for y = 0 to y = 0.16 between 800 and 1700 K at one bar total pressure.

9.14 Activity of the Fe component in wustite for y = 0 to y = 0.16 between 800 and 1700 K at one bar total pressure.

9.15 The function $\overline{S}(O_2)-\overline{S}^\circ(O_2)$ in wustite for y = 0 to y = 0.16 between 800 and 1700 K at one bar total pressure.

9.16 The function $\overline{H}(O_2)-\overline{H}^\circ(O_2)$ in wustite for y = 0 to y = 0.16 between 800 and 1700 K at one bar total pressure.

9.17 The function $\overline{G}(O_2)-\overline{G}^\circ(O_2)$ in wustite for y = 0 to y = 0.16 between 800 and 1700 K at one bar total pressure.

9.18 Activity of the O_2 component in wustite for y = 0 to y = 0.16 between 800 and 1700 K at one bar total pressure.

9.19 The function $\overline{S}(FeO)-\overline{S}^\circ(FeO)$ in wustite for y = 0 to y = 0.16 between 800 and 1700 K at one bar total pressure.

9.20 The function $\overline{H}(FeO)-\overline{H}^\circ(FeO)$ in wustite for y = 0 to y = 0.16 between 800 and 1700 K at one bar total pressure.

9.21 The function $\overline{G}(FeO)-\overline{G}^\circ(FeO)$ in wustite for $y = 0$ to $y = 0.16$ between 800 and 1700 K at one bar total pressure.

9.22 Activity of the FeO component in wustite for $y = 0$ to $y = 0.16$ between 800 and 1700 K at one bar total pressure.

9.23 Thermodynamic properties of wustite (calorimetric sample, $Fe_{0.947}O$) between 200 and 1700 K at a total pressure of one bar.

9.24 Log a(Fe) and related properties in wustite (calorimetric sample, $Fe_{0.947}O$) between 800 and 1700 K at a total pressure of one bar.

9.25 Log $a(O_2)$ and related properties in wustite (calorimetric sample, $Fe_{0.947}O$) between 800 and 1700 K at a total pressure of one bar.

9.26 Log a(FeO) and related properties in wustite (calorimetric sample, $Fe_{0.947}O$) between 800 and 1700 K at a total pressure of one bar.

Table 9.01 through 9.26 near here.

CHAPTER 10

RECOMMENDED STANDARD ELECTROCHEMICAL POTENTIALS AND RELATED DATA

The following tables supply the recommended standard electrochemical potentials and oxygen fugacities for the nine buffer reactions (equations 3.1 through 3.9). The 2-sigma confidence limits are given at 298.15 K and at each 250-K isotherm. The confidence limits were calculated from the variance-covariance matrix resulting from the least-squares fitting of the mathematical model to the thermodynamic data and to all reaction data and will be equal to or less than that estimated from the tables given in Chapter 8. For details of the calculation of the confidence limits, refer to Appendix C or to Clifford (1973). The 2-sigma limit was used because the results of the evaluation depend primarily on the evaluated reaction data and only to a minor extent on the auxiliary data for which confidence limits could not be evaluated properly.

Figure 10.1 near here.

Figure 10.1 supplies a quick graphic display of the relative positions of the oxygen buffers to each other. On Figure 10.1 one will note an anomalous change in the slope of the SiO_2-Fe_2SiO_4-Fe_3O_4 buffer curve. The potential for the corresponding reaction

$$2\ Fe_3O_4(\text{magnetite}) + 3\ SiO_2(\text{quartz}) = 3\ Fe_2SiO_4(\text{fayalite}) + O_2(g) \qquad 10.01$$

appears to be linear with temperature above 900 K. The curvature is most noticeable between 750 and 850 K. When one considers the reaction, one must note that there are 2 moles of magnetite and 3 moles of quartz on the reactant side of equation 10.1. These phases have a combined entropy contribution of 37.3 J/(mol K) for the reaction between 750 and 850 K. The phases in the product of the reaction have no significant anomalies. The magnetic anomaly for magnetite and the first- and second-order anomalies associated with the alpha-beta quartz inversion are the causes for this anomalous change in slope. Other reactions where magnetite, quartz, bunsenite, hematite, iron, or nickel are present also have changes in slope but the curvature is not so obvious (1) because of the scale of the plot, (2) because the number of moles of the phase involved is small, or (3) the entropy changes are not as significant as for the buffer reaction in equation 10.1. When one reduces electrochemical potentials to linear equations, one must also look at the properties of the phases in the reaction and the accuracy needed from the algebraic representation of the potential.

On some tables, the change in volume for the solids was supplied at one bar. This allows a quick estimate of $\Delta_r G(T,P)$.

$$\Delta_r G(T,P) = \Delta_r G^\circ(T,1.0) + 0.1 \int_1^P \Delta_r V \, dP \qquad 10.02$$

At elevated pressure, the reactions are "vapor absent". That means that the pressure of oxygen gas is less than the total pressure and the activity of oxygen is controlled by the equilibrium between the solid phases only. Therefore,

$$\int_1^P \Delta_r V \, dp = \int_1^P \Delta_r V(\text{solids}) \qquad 10.03$$

As an example of the calculation of the properties at elevated pressure and temperature, consider the following reaction at 750 K and 5,000 bars.

$$2\ \mathrm{NiO(bunsenite)} = 2\ \mathrm{Ni(s)} + \mathrm{O_2(g)} \qquad 10.04$$

If one integrates the equations for volume of Ni and NiO from 1 bar to 5000 bars,

$$\Delta_r G(750{,}5000) = 336{,}724\ \mathrm{J/mol} \qquad 10.05$$

and

$$\log a(\mathrm{O_2}) = -23.45_1 \qquad 10.06$$

If column 6 of Table 10.3 is used to estimate equation 10.02,

$$\Delta_r G(750{,}5000) = 341{,}211 + 0.1\cdot(-8.9967)\cdot(5000-1) \qquad 10.07$$

$$= 336{,}713\ \mathrm{J/mol} \qquad 10.08$$

and

$$\log a(\mathrm{O_2}) = -23.44_0 \qquad 10.09$$

The difference between the two methods of calculation are 11 J/mol and 0.01_0 in $\Delta_r G(750{,}5000)$ and $\log a(\mathrm{O_2})$, respectively. The first method is more accurate. However, at 5,000 bars, the improvement is not needed for most geological applications. The priciple application of the first method of calculation will be the evaluation of the thermochemical data for other solids at high pressures or where large volume changes are developed because one does not want to introduce systematic errors if they can be avoided.

The tables are arranged in the order listed below.

Table	Reaction
10.1	2 Cu_2O (cuprite) = 4 Cu(s) + O_2(g)
10.2	4 CuO (tenorite) = 2 Cu_2O (cuprite) + O_2(g)
10.3	2 NiO (bunsenite) = 2 Ni(s) + O_2(g)
10.4	2 $Fe_{1-y}O$ (wustite) = 2(1-y) Fe(s) + O_2(g)
10.5	.5 Fe_3O_4 (magnetite) = 1.5 Fe(s) + O_2(g)
10.6	Fayalite = 2 Fe(s) + SiO_2 (quartz) + O_2(g)
10.7	(1-2y)/(1-4y) Fe_3O_4 (magnetite) = 3/(1-4y) $Fe_{1-y}O$ (wustite) + O_2(g)
10.8	2 Fe_3O_4 (magnetite) + 2 SiO_2 (quartz) = 3 fayalite + O_2(g)
10.9	6 Fe_2O_3 (hematite) = 4 Fe_3O_4 (magnetite) + O_2(g)

Table 10.1 through 10.9 near here.

CHAPTER 11

RECOMMENDATIONS FOR FUTURE RESEARCH

Introduction

In preparing this report several topics for future research became evident. They are as follows:

- Develop a procedure to insure that experimental data are not lost in the publication process.
- Carefully study wustite below 1000 K by the collection of the following data:
  - a. calorimetric measurements of additional samples, especially at higher values of excess oxygen,
  - b. compositional data defining the stability field for wustite,
  - c. time-temperature-transformation (ttt) studies, especially at temperatures less than 850 K at ambient pressures,
  - d. ttt studies at elevated temperatures,
  - and e. oxygen or iron potentials at elevated pressures as a function of composition and data that defines the shape of the wustite stability field.
- Analyse the available data for MO-FeO-O_2 systems at low Fe contents to derive the best form of the log $a(O_2)$-x function at low values of x and at low activities of O_2. MO might be MgO, NiO, CoO, or MnO.

- Measure volumetric data for all phases at elevated pressures and temperatures.
- Experimentally test the extrapolations of the buffer potentials to higher pressures.
- Develop a procedure to insure that the experimentalist will characterize the sample used in research as to purity and crystal structure.

Publication of Experimental Data

Develop a procedure to insure that experimental data are not lost in the publication process.

It is unfortunate that editors and authors are being pressured to reduce manuscript size and most unfortunate that they choose to do so through the elimination of critical experimental data. An experimental observation is a fact. It will not change with time or place if it is recorded correctly. Interpretations and evaluations are subject to the current scientific understanding. That understanding is subject to change. Interpretations may change. Critical constants may be revised. Evaluation methods will improve. The experimental data, on the other hand, are constant and are the proper base for publication and for evaluation of thermodynamic data. In reality, the conclusions of a paper are as so much arm-waving. They become significant only if they stand the test of time through repeated analysis of the contained data and of additional data.

In an earlier discussion the presentations of experimental heat capacity data for bunsenite as smoothed graphs were cited. It was unfortunate that the authors did not supply the experimental details. As for thermodynamic usefulness, their man-years of research were greatly diminished and the research funds were lost because they chose to give summaries of their work and not the real data. The studies for bunsenite were not isolated cases. Too many studies and too many man-years of effort are left uncited here because the experimental data were given only as a graph that had been reduced in the publication process to the author's obscurity.

Equations, though useful, are not a satisfactory substitute for experimental data. Any smoothing process biases the results. Because data were smoothed using stated or unstated techniques or constants, the correct accuracy of the thermodynamic evaluation was compromised. If the smoothed data are a significant component of the body of data being evaluated, then, to that degree, the whole evaluation would be biased.

In summary, the authors should publish the experimental data if they want their efforts to be cited and included in thermodynamic evaluations properly.

Study of Wustite Below 1000 K

Carefully study wustite below 1000 K by the collection of the following data:

a. calorimetric measurements of additional samples, especially at higher values of excess oxygen.

b. compositional data defining the stability field for wustite.

c. time-temperature-transformation (ttt) studies, especially at temperatures less than 850 K at ambient pressures.

d. ttt studies at elevated ~~temperatures~~ pressures.

e. oxygen or iron potentials at elevated pressures as a function of composition and data that defines the shape of the wustite stability field.

Careful research on wustite at temperatures below 1000 K are needed to improve and expand the body of knowledge on this important oxide phase. One of the conclusions of this study was that the composition of wustite at the breakdown temperature or 839.15 K was $Fe_{0.917}O$. The quality of the data on the composition of wustite below 1000 K was poor. Equilibrium between gas mixtures and solids is slow at these temperatures and electrobalance techniques to measure composition fail because the solids are not at equilibrium. Electrochemical studies require longer run times and there is more opportunity for contamination and biased results.

Calorimetry of additional samples are needed, particularly at higher values of excess oxygen than in the calorimetric sample $Fe_{0.947}O$. Such data will supply the best means of identifying the properties of wustite in the metastable region at low temperatures.

A careful study of the stability limits of wustite below 1000 K and the breakdown temperature near 839 K is needed. The thermodynamic data and the physical measurements do not match the estimated compositions developed by Darken and Gurry (1945, 1946). The data are consistent with the limited observations by Hoffmann (1959) among others. This should be coordinated with the ttt studies below.

In developing a study of the physics and chemistry of wustite, attention should be paid to the complexities of order-disorder in the wustite phase. As recommended by Hazen and Jeanloz (1984), time-temperature-transformation (ttt) analyses of several wustites would be an important step. More effort using *in situ* phase identification and characterization should be made during the course of the chemical experiments. The nature of the intermediate breakdown products will yield clues as to the positions of the metastable extensions of the iron-wustite and wustite-magnetite boundaries. The data will also improve the interpretation of the calorimetric data and the electrochemical data in this temperature region.

Additional ttt studies at elevated pressures are needed. The compositional shape of the wustite stability field at elevated pressures is largely unknown. Some data are available for cell edges of wustites coexisting with iron (Simons and Seifert, 1979). What about the wustite-magnetite boundary? Hazen and others (1981) have detected a non-ideal elastic behavior at elevated pressures. What is the nature of this behavior? Is this the cause of the smaller quenched cell data for "FeO" synthesized at 775°C (1048 K) and pressures greater than 50 kb as reported by Akimoto (1972)?

Detailed thermochemistry is needed for wustite solid solutions at elevated pressures. What are the oxygen (or iron) potentials as a function of composition at elevated pressure? How are these potentials affected by the non-ideal elastic behavior?

Extensi~~t~~on to Other Systems

Analyse the available data for $MO-FeO-O_2$ systems at low Fe contents to derive the best form of the log $a(O_2)-x$ function at low values of x and at low activities of O_2. MO may be MgO, NiO, CoO, or MnO.

By exten~~t~~ding the analysis to solid solutions containing components such as MgO, NiO, CoO, or MnO, the mathematical model may be adjusted and improved to include lower excess oxygen contents with greater confidence. At ambient pressure, the data are useful for metallurgical research and laboratory studies. At higher pressures, the data would describe the properties of a potentially important phase in the mantle, namely, magnesiowustite.

Volumetric Data

Measure volumetric data for all phases at elevated pressures and temperatures.

In the real world increasing attention needs be given to volumetric data of all types. Especially in the geological sciences, but also for some industrial applications, thermodynamic predictions at elevated pressures are being used. These predictions cannot be made accurately without reasonably good descriptions of the molar volumes as a function of temperature and pressure. Preparation of thermodynamic correlations and compilations is a service function. By including molar volumes and the coefficients of volume expansion and of volume compression, the standard compilations are more useful. By including the volumetric properties within the evaluation scheme, accuracy and applicability of the standard compilations are increased. Benefits are returned to the evaluator in the form of support. But the evaluator cannot work alone. The experimenter must also consider the measurement of molar volumes, expansivities, and compressibilities as part of the necessary phase characterization. The more careful and thorough the research is, the more lasting the products will be.

Experimental Tests of Extrapolation to High Pressure

Experimentally test the extrapolation of the buffer potentials to higher pressures.

In the data evaluated here, the oxidation of fayalite to magnetite and quartz by $H_2O(g)$, the reduction of bunsenite by $H_2(g)$, and the electrochemical potential difference between the Ni-NiO buffer and the magnetite-hematite buffer were studied at high pressures. For the oxidation of fayalite and the reduction of bunsenite, the pressure did not exceed 2 kilobars. For the potential differences in the Ni-NiO and the magnetite-hematite buffers, the data to nearly 7 kilobars are acceptable but the data at 34 kilobars are in error. Yet, the application of much of the thermodynamic data will be used to evaluate experimental data on silicates at pressures as high as 30 kilobars or more. It is recommended that tests be set up which provide a check the equilibria and the volumetric data. By such tests, closure of the thermodynamic cycle as a function of pressure may be achieved.

Characterization of Samples

Develop a procedure to insure that the experimentalist will characterize the sample used in research as to purity and crystal structure.

Some difficulties were encountered in this study where the author reported experimental results but did not identify the polymorph of a chemical that was present during the experiment. In particular, this was common for studies dealing with SiO_2. Authors only reported the chemical formulas but did not identify the phase present. Because both quartz and cristobalite will persist well beyond the phase stability limits, the identity of the phase is important. Fortunately, the Gibbs energy difference between quartz and cristobalite is small in the temperature region of the experiments. Other factors such as lack of chemical equilibrium contributed most of the uncertainty for the silicates in this study.

However sample purity for fayalite is believed to be the major cause of error in the measurement of the molar volumes. The presence of manganese in small amounts in the natural samples usually leads to larger molar volumes. More careful identification of the chemical composition of the wustites used in electrochemical studies, both before and after the experiments, would have shown that there were changes in the composition caused by the exchange of oxygen.

CHAPTER 12

SUMMARY

A critical review was made of the experimental data relating to the solid oxygen buffers copper-cuprite, cuprite-tenorite, nickel-bunsenite, iron-wustite, iron-magnetite, wustite-magnetite, magnetite-hematite, quartz-fayalite-iron, and quartz-fayalite-magnetite. The review included the available data for molar volume, expansivity, compressibility, heat capacity, entropy, and heat contents for each oxide and silicate in the list. The review also included the data relating to 44 chemical reactions where enthalpies and Gibbs energies of reaction, equilibrium constants, and electrochemical potentials were measured and reported. The review included a considerable effort to identify the phase relations for wustite, $Fe_{1-y}O$ or FeO_{1+x}, as a function of temperature, pressure, composition, coexisting phases, and activities of oxygen and iron.

The following products are the result:

(1) recommended thermodynamic data for the phases tenorite (CuO), cuprite Cu_2O), bunsenite (NiO), ferrous oxide (FeO), magnetite (Fe_3O_4), hematite (Fe_2O_3), fayalite, (Fe_2SiO_4,s1), and the diferrous silicate spinel (Fe_2SiO_4,s2),

(2) recommended thermodynamic data for the wustite solid solution ($Fe_{1-y}O$ or FeO_{1+x}). This included the molar volume,

expansivity, compressibility, heat capacity, entropy, heat content, entropy of formation, enthalpy of formation, Gibbs energy of formation, partial molar quantities for Fe, FeO, and O_2, and the activities of Fe, FeO, and O_2 as a function of both "y" and "x".

(3) recommended standard electrochemical potentials at one bar total pressure for the nine oxygen buffer reactions represented by the above phase assemblages.

and (4) recommendations for future research that is necessary to improve the thermodynamic correlations.

CHAPTER 13

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APPENDIX A

EVALUATION OF THE REACTION DATA

Introduction

In Chapter 7, a summary of the data for the reactions included in this optimization was supplied by phase. For example, refer to Tables 7.19 through 7.26 and the associated text. The details supporting the rows of data on the tables are supplied in this appendix by reaction.

Evaluation Procedures

Introduction

A reader may get caught up in the details presented here. Therefore, it should be stated again that the conclusions and data in Chapters 8 through 11 are the results of evaluating all data simultaneously using a least squares technique and an internally consistent mathematical model for the thermodynamic properties.

The process of evaluating a specific study of a chemical reaction began with the reading of the author's description of the experimental method and the treatment of the data. If the experimental method was faulty, the data were flagged and were given zero weight. One example of a faulty experimental method was the use of sandwich-type stacking of a mixture of one buffer assemblage, a wafer of doped zirconia electrolyte, and a mixture of another buffer assemblage (Kiukkola and Wagner, 1957). The atmosphere that develops around one buffer assemblage could bypass the electrolyte wafer and contaminate the atmosphere around the second assemblage. The experiment becomes biased and yields data indicating an anomalously low potential. If the electrochemical equilibration is rapid, the run times are short, and the ionic conductivity of the electrolyte is high, the experiments may produce data approaching the correct results. There are many experiments that did not contain this possible flaw. Therefore, the flawed data were dropped by assigning zero weight to the data.

A second reason for modifying weights of a set of data, even to the assignment of zero weight, was the common practice of converting the experimentally measured data to some other derived property. An example was the conversion of electrochemical potentials to log $a(O_2)$ values without the explicit statement as to what conversion factors were used. Without knowing which values were used for R, F, or ln(10), this evaluator was left with only one choice, lower the stated precision (increase the absolute magnitude of the precision) by an appropriate amount depending upon the range of possible conversion factors. An example was the common use of "2.303" for ln(10). This represents a systematic error in the converted data of 0.018 percent. Often, this is larger than the stated precision.

Another practice used by experimentalists is to report the results for a reaction where a second potential of unknown magnitude was removed. An example was the experimental research by Matsushita and Goto (1963). Refer to Table A.03 and the associated text in this appendix. Such data sets were given zero weight.

The next step was the comparison with the available calorimetry for each phase in the reaction. The disagreements among the calorimetry for bunsenite (NiO), for magnetite (Fe_3O_4), and for the reaction data were noted early in the process. As the evaluation progressed and various potential reasons for the disagreements were eliminated, it became apparent that:

(1) the calorimetric entropy, $S^\circ(298)-S^\circ(0)$, of bunsenite (King, 1957) was high,

and (2) the calorimetric data for magnetite above room temperature was both too high (Grønvold and Sveen, 1974), and too low (Coughlin and others, 1951).

The final step was the comparison of data describing the many reactions with each other. At this step, data were either kept or eliminated depending upon one or more of the following:

(1) internal agreement among the data sets,

(2) third-law $_{r}H^\circ(298)$-temperature plots for specific data sets,

(3) known problems related to lack of equilibration among gases or solids,

and (4) systematic errors in a set of unrelated experiments using the same experimental procedure and published by the same author.

Internal agreement

An example of good internal agreement is the correlation among data for reactions given by equations A.01, A.02, and A.03, below. All data were measured electrochemically.

Cu_2O(cuprite) + Ni(s) = 2 Cu(s) + NiO(bunsenite) A.01

2 Cu(s) + 3 Fe_2O_3(hematite) = Cu_2O(cuprite) + 2 Fe_3O_4(magnetite) A.02

Ni(s) + 3 Fe_2O_3(hematite) = NiO(bunsenite) + 2 Fe_3O_4(magnetite) A.03

Where there is good agreement among a set of related reactions such as these three, adjustments of the properties of one phase cannot be done without determining what effect the adjustment will have on the other phases. This will be discussed in the text associated with Tables A.08, A.27, and A.28, later in this appendix.

Third-Law $\Delta_r H°(298)$-Temperature Plots

Figure A.02, an enthalpy-temperature plot for the reaction given by equation A.04 and found on page A-7, is a good example of the use of these plots.

$$2\ Cu(s) + 0.5\ O_2(g) = Cu_2O(\text{cuprite}) \qquad A.04$$

One may readily observe which sets are consistent with the calorimetry and others reaction data and which sets are divergent. The consistent sets plot along the horizontal line calculated from the fitted model. The divergent sets may plot elsewhere on, or even off, the plot. These details are not always obvious on the plots of log K° (Figure A.01 found on page A-7).

Equilibration

Equilibration among the gas mixtures that were used to control the oxidation state, was a problem in some experiments. All data derived from the use of the H_2-CO_2 gas mixtures were given zero weight in the fitting process. This particular mixture does not equilibrate quickly because equilibrium among 5 gaseous species (H_2, H_2O, O_2, CO_2 and CO) must be attained. To add to the problem, the experiments required that the equilibrium must be attained in a thermal gradient in a flowing fluid.

Most of the data for silicate reactions indicate that silica, either as quartz or cristobalite, and fayalite equilibrates slowly. A good example of lack of equilibrium in silicate experiments is shown on Figures A.70 and A.71 in this appendix.

Systematic Errors

Though it was not readily obvious at the outset, all reactions studied electrochemically by Myers and Eugster (1983) gave lower potentials (higher activities of oxygen) than other studies for the same reactions. All reactions in this study ~~was~~ were given zero weight in the final optimization.

Another example of a systematic error is the research reported by Ariya and Yakovleva (1970). They reported electrochemical potentials between wustite of fixed compositions and the iron-wustite phase assemblage. They also measured the oxygen-potential difference between the wustite-magnetite and the iron-wustite phase assemblage. The latter data are in good agreement with other studies. Refer to Figure A.40 in this appendix. However, the other data indicate that the wustites of constant composition contained higher concentrations of oxygen than the authors reported. Refer to Figure 7.46.

Control of the oxidation state in unbuffered wustite samples was a major problem in electrochemical experiments. As can be found on Table A.10, none of the resulting data were used in the final optimization. None of the data were consistent with the expected potentials for the compositions reported by the authors.

Data Ordered By Reaction

Introduction

The list of reactions is a confusing array. In order to bring some order to that array, the available data, by reaction, are presented in the order given below.

Reactions with Cu_2O.

Reactions with CuO without and with Cu_2O.

Reactions with NiO without and with Cu_2O and CuO.

Reactions with FeO without and with Cu_2O, CuO, and NiO.

Reactions with Fe_3O_4 without and with Cu_2O, CuO, NiO, and FeO.

Reactions with Fe_2O_3 without and with Cu_2O, CuO, NiO, FeO, and Fe_3O_4.

Reactions with Fe_2SiO_4 without and with Cu_2O, CuO, NiO, FeO, Fe_3O_4 and Fe_2O_3.

$2\ Cu(s) + 0.5\ O_2(g) = Cu_2O$(cuprite)

Table A.01 contains a summary of the available data for this reaction. Figure A.01 shows the observed data and the calculated values. For each experimental observation, the enthalpy of reaction at 298.15 K was calculated and plotted on Figure A.02.

The fitted $\Delta_r H°(298)$ is in good agreement with the results of the combustion calorimetry reported by Mah and others (1967). The research by Matsushita and Goto (1963) were given zero weight in the evaluation because auxiliary data used by them were unavailable. The research of Peters (1983) and of Kodera and others(1968) were also given zero weight. Figure A.02, part a shows that the two studies depart significantly from the other studies. In particular, the data of Kodera and others (1968) were not in agreement with the available calorimetry. The early research by Treadwell (1916), using an unreliable solid electrolyte, was also given zero weight in the final evaluation. The other emf studies are internally consistent and also consistent with the calorimetric data for Cu_2O, such as heat capacity, entropy, and relative heat contents.

Figures A.01 and A.02 and Table A.01 near here.

Cu_2O(cuprite) + CO(g) = 2 Cu(s) + CO_2(g)

Table A.02 contains a summary of the available data for this reaction. The data of Peters and Mann (1958) are shown on Figure A.03 along with the fitted curve. The calculated enthalpies of reaction at 298.15 K for their data are shown on Figure A.04 as a function of the temperature of observation. As with their study on the reduction of bunsenite with CO(g), these data indicate the oxide is less stable than indicated by other studies. The data were given zero weight in the evaluation.

Figures A.03 and A.04 and Table A.02 near here.

$2\ Cu(s) + O_2(g) = 2\ CuO$(tenorite)

Table A.03 contains a summary of the available data for this reaction. Mah and others (1967) determined the enthalpy of formation of tenorite by combustion calorimetry. The fitted functions are in good agreement with the experimental observation.

The derived results by Matsushita and Goto (1963) are shown on Figure A.05 and Figure A.06. The data have an anomalous slope that was caused by use of erroneous constants in the data reduction by Matsushita and Goto. The data were given zero weight.

Figures A.05 and A.06 and Table A.03 near here.

Cu_2O(cuprite) + 0.5 O_2 = 2 CuO(tenorite)

Table A.04 contains a summary of the available data for this reaction. Figure A.07 shows the observed and calculated values. For each experimental observation, the enthalpy of reaction at 298.15 K was calculated and plotted on Figure A.08. Again, as for the Cu-Cu_2O equilibria, the research data of Peters (1983), of Kodera and others (1968), and of Treadwell (1916) were given zero weight in the final evaluation. From examination of the enthalpy-temperature plots, it was evident that the mass-spectrometric data by Norton (1955) were also not consistent with the calorimetric data. Norton's study was given zero weight.

Figures A.07 and A.08 and Table A.04 near here.

$Ni(s) + 0.5\ O_2(g) = NiO$(bunsenite)

The Ni-NiO equilibrium has been the subject of extensive experimental research because the phases are important in metallurgy, solid state physics, and geochemistry. Table A.05 contains a summary of the available data for this reaction. Figure A.09 shows the experimentally observed data and the fitted curves. In addition, the enthalpies of reaction calculated for each observation are shown on Figure A.10.

The research of Barbi (1964a), Berglund (1976), Kazenas (1969), Moriyama and others (1969), Moser and others (1975), Myers and Gunter (1979), Saito and others (1972), Schwab and Kuestner (1981), Tran and Brungs (1980), and Taylor and Schmalzreid (1964) were given zero weight because of excessive drift as shown on the enthalpy-temperature plots. The research of Huebner and Sato (1970) were given zero weight because the enthalpy-temperature plot showed the data to be less precise. The data of Treadwell (1916) were given zero weight because the data depended on the performance of an unreliable solid state electrolyte. The balance of the data are consistent with the combustion calorimetry of Boyle and others (1954) and the new heat capacity data by Hemingway (1984) but inconsistent with the entropy of King (1957). The entropy was rejected and a revised, slightly lower entropy of 36.70±0.33 J/(mol K), as obtained by the final evaluation, was accepted.

Figures A.09 and A.10 and Table A.05 near here.

$NiO(bunsenite) + CO(g) = Ni(s) + CO_2(g)$

Table A.06 contains a summary of the available data for this reaction. The reported experimental data for the above equilibrium are given on Figure A.11. The enthalpies of reaction at 298.15 K calculated from the high-temperature observations are plotted as a function of temperature on Figure A.12 . The early research of Fricke and Weitbrecht (1942) and the work of Navrotsky and Muan (1970) and of Peters and Mann (1958) were given zero weight. The enthalpy-temperature plots show these data to be divergent.

Figures A.11 and A.12 and Table A.06 near here.

NiO(bunsenite) + $H_2(g)$ = $Ni(s)$ + $H_2O(g)$

Table A.07 contains a summary of the available data for this reaction. The experimental data of Pease and Cook (1926) and of Rau and Guedes de Carvalho (1973) are shown on Figure A.13 and the calculated enthalpies of reaction at 298.15 K as a function of the temperature of observation are shown on Figure A.14. It is apparent that equilibrium was not obtained at temperatures below about 720 K. Those data below 720 K were given zero weight in the final evaluation. Otherwise the results are in acceptable agreement with the other ractions above.

It should be noted that Gunther and others (1979) made equilibrium measurements at 2 kb total pressure. The enthalpies of reaction at 298.15 K were calculated after the Gibbs energies of reaction were reduced to 1.0 atm using the available data for the molar volumes of Ni and NiO.

The experimental data reported by Babushkin and others (1971) could not be interpreted. The equilibrium constants, as given, were 1.5 to 2.0 log units less positive than the calculated values.

Figures A.13 and A.14 and Table A.07 near here.

Cu_2O(cuprite) + Ni(s) = 2 Cu(s) + NiO(bunsenite)

The above reaction is the net for the potential difference between the copper-cuprite and the nickel-bunsenite assemblages. Table A.08 contains a summary of the available data for this reaction. Figures A.15 shows the experimental data for this reaction. The enthalpies of reaction for each observation are plotted on Figure A.16.

The experimental results of Bonnet and Perrin (1978), Bugden and Pratt (1970), Moriyama and others (1969), Moser and others (1975), Ramakrishnan and others (1975), Trumm (1971), and Vasileva and others (1975) were given zero weights in the final evaluation. The data are consistent but the sandwich-type technique was used to measure the electrochemical potentials. The balance of the observations are in good agreement with each other and with other data contained in the evaluation.

The study by O'Neill (1987) was received after the study was completed. The fitted thermochemistry is consistent with the data from that study. This is noteworthy. The potentials that O'Neill (1987) supplied for the oxygen potential difference between the quartz-fayalite-magnetite and the copper-cuprite buffers are not consistent with other available data. (Refer to Table A.43 and the associated text.) If O'Neill's (1987) work on fayalite is correct, then both cuprite and bunsenite must be adjusted proportionally. The preponderance of data for the copper-cuprite and the nickel-bunsenite equilibria do not support any adjustment.

Figures A.15 and A.16 and Table A.08 near here.

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2 CuO(tenorite) + Ni(s) = Cu_2O(cuprite) + NiO(bunsenite)

Table A.09 contains a summary of the available data for this reaction. Figure A.17 shows the experimental observations of Charette (1967) for the above reaction. The calculated enthalpies of reaction at 298.15 K are given on Figure A.18. While there was some indication of systematic offset (about 0.001 volts), it was not significant and the calculated values are within the precision of the experimental data.

Figures A.17 and A.18 and Table A.09 near here.

$2\ FeO(wus,sln) = 2\ Fe(wus,sln) + O_2(g)$

Wustite is a solid solution having the halite structure but also having cation defects and cation interstitials. In this report, both formula are used. The relation between x and y is

$$1 + x = \frac{1}{1 - y} \qquad \text{A.05}$$

As a first approximation, thermodynamic quantities correlate with x better than with y. For example, equation A.06 gives the empirical relation between $\log f(O_2)$ and x, the moles of excess oxygen in wustite.

$$\log f(O_2) = r(T) + s(T)\ x \qquad \text{A.06}$$

Equation A.06 is basic to the thermodynamic data developed here for FeO and for the wustite solid solution. It is with some care that the functions r(T) and s(T) were chosen. The available studies where $\log f(O_2)$ was measured as a function of composition at constant temperature were fit by least-squares techniques to get the slopes and intercepts for each isotherm. Related data, such as reported CO_2/CO values, were converted to $\log a(O_2)$ values prior to this trial fitting of the isotherms. The values for the intercepts and for the slopes were ploted on Figures A.19 and A.20, respectively.

Figures A.19 and A.20 near here.

Based on the scatter of slopes shown on Figure A.20, the data supplied by Janowski and others (1973, 1974) were given zero weight. The slopes and intercepts scatter excessively and the measurements probably do not represent true equilibrium. The same is true of the studies by Myers and Eugster (1983) and Barbero (1981).

The optimization produced the following fitted functions for r(T) and s(T).

$$r(T) = 5.36060\ (1 + \ln T) - 0.71074 \cdot 10^{-3}\ T - (3.57076 \cdot 10^{4})/T + 45.9213 \qquad 7.49$$

$$s(T) = 4.39866 \cdot 10^{-3}\ T + 17.3524 \qquad 7.50$$

Use of a function linear in temperature for s(T) was important. The useable data scattered too much to justify a more complex function. Also, the choice of a function linear in reciprocal temperature would lead to log $a(O_2)$-x relation with a low slope or even a negative slope at low temperatures. A negative slope is not physically possible, even in the metastable region at low temperatures. Giddings (1972) used the linear reciprocal temperature relation. The calculated slope was negative below 264 K. Knacke (1983) used Gidding's data in his model for the wustite solid solution and his model contains the same flaw. The analyses provided by Giddings (1972) or by Knacke (1983) cannot be used to derive the thermodynamic properties of wustite in the metastable region below the isobaric invariant point of 839 K.

The validity of equation A.06 for modelling the solid solution was tested using the following chemical reaction. Where data were reported using other chemical reactions, the appropriate conversions were made to reduce all data to observed log $a(O_2)$ values.

$$2\ \mathrm{FeO(wus,sln)} = 2\ \mathrm{Fe(wus,sln)} + \mathrm{O_2(g)} \qquad \text{A.09}$$

At equilibrium,

$$\Delta_r G^\circ(T) = -R\,T\,\ln(10)\,[2 \log a(\mathrm{Fe}) + \log a(\mathrm{O_2}) - 2 \log a(\mathrm{FeO})] \qquad \text{A.10}$$

Using the third-law enthalpy calculation given in Chapter 7,

$$\begin{aligned}\Delta_r H^\circ(298) &= -\,R\,T\,\ln(10)\,\log a(\mathrm{O_2}) \\ &\quad -\,R\,T\,\ln(10)\,[2 \log a(\mathrm{Fe}) - 2 \log a(\mathrm{FeO})] \\ &\quad -\,T\,[2\,\mathrm{gef}^\circ(\mathrm{Fe}) + \mathrm{gef}^\circ(\mathrm{O_2}) - 2\,\mathrm{gef}^\circ(\mathrm{FeO})] \qquad \text{A.11}\end{aligned}$$

The reported (or converted) value for each observation was combined with the calculated activities for Fe and FeO and the Gibbs energy functions to calculate $\Delta_r H^\circ(298)$. Figures A.21, part a through A.21, part y show the third-law enthalpy-composition plots ordered alphabetically by author. An open circle (o) on the plots show that the datum represented by the symbol was given zero weight. A plus sign within the circle (⊕) shows that the datum was given a weight appropriate for the observation. Because the enthalpy-composition plots contained more detail, they were found to be more useful than the log $a(\mathrm{O_2})$-composition plots. The latter plots are not supplied here.

The data are summarized on Table A.10. The first half of the table is a summary of the data used in the optimization. The second half gives a summary of the remaining data that were given zero weight. The studies that were given zero weight, other than those by Barbero and others (1981), Janowski and others (1973), and Myers and Eugster (1983) were shown to be inferior by the scatter and trend of the enthalpies. The data reported by Marion (1955) were used but the precision was lowered (absolute magnitude was increased) by a factor of 4. These data, particularly the values reported for temperatures greater than 1250 K (14 values), might be in error due to Soret effect. This effect develops in a gas mixture where there is a considerable contrast in the molecular weight of the components and where the mixture is contained in a thermal gradient. Thermal diffusion will cause the gases to separate somewhat by density and the resulting mixture is not homogeneous. Removal of these suspect values would not change the results because they had been given a much lower weight and because there are other data in the same temperature range that have higher precision and therefore more weight.

Figure A.21, part a through A.21, part y and Table A.10 near here.

2 FeO(wus,sln) = 2 Fe(s) + O_2(g)

Figure A.22 is a plot of the reported data and of the fitted equation. Figure A.23 shows the calculated enthalpies of reaction at 298.15 K plotted as a function of the temperature of observation. In Table A.11, the sources marked with an asterisk (*) were used during the final fitting process.

The plots of data, in particular, the plots of the enthalpy of reaction as a function of temperature are not particularly convincing that the best solution was obtained for this reaction. One must keep in mind that the fugacity of oxygen is not something that cannot be observed directly at the levels reported except by electrochemical techniques. With electrochemical techniques, much care must be taken to prevent contamination by O_2 gas which will diffuse through the ceramic electrolyte slowly. Unfortunately, many of the authors did not report the experimental data but choose to supply the derived fugacities using constants and auxiliary data not given in the articles. Other reactions to be discussed will show that the fitted functions are indeed the correct functions.

Figures A.22 and A.23 and Table A.11 near here.

$FeO(wus,sln) + CO(g) = Fe(s) + CO_2(g)$

The experimental data are cited on Table A.12 and are plotted on Figure A.24. The calculated enthalpies of reaction at 298.15 K for each observation are plotted as a function of the temperature of observation on Figure A.25. The results of Peters and Mann (1959) differ from the data reported in 1958 only in round off of the fitted coefficients. Therefore both reports were given zero weight. The research by Chaudron (1921) were also given zero weight. The reversed data are scattered and not critical enough to restrict the solution.

The data of Vallet and Raccah (1965) average more oxidizing than the fitted function. This persisted even after a correction of -0.04 in log K was made because the CO_2/CO equilibria used in this study was 0.04 units more negative than the compilation of Elliott and Gleiser (1960) that was used by Vallet and Raccah to convert their CO_2/CO ratios to oxygen fugacities. Unfortunately the ratios of CO_2/CO used in the experiments were not reported. Other constants such as the ideal gas constant R or the numerical value for "ln(10)" may have departed systematically. Much of the graphed data are more reduced than the fitted function. If the data of Vallet and Raccah (1965) were removed it might be argued that the data for $CO_2(g)$ and for CO(g) were in error. Such an assumption is not supported by other reactions where CO_2-CO gas mixtures were used to control the experiments or where H_2O-H_2 gas mixtures were used.

Matsubara's (1922) data has an anomalous trend and were given zero weight. The study by Kondakov and Wan (1958) was obtained after the optimization was completed and therefore had zero weight.

Figures A.24 and A.25 and Table A.12 near here.

$FeO(wus,sln) + H_2(g) = Fe(s) + H_2O(g)$

The experimental data cited in Table A.13 are shown on Figure A.26. The calculated enthalpies of reaction at 298.15 K are plotted on Figure A.27 as a function of the temperature of observation. Based on the enthalpy-temperature plots, the research Brit~~s~~zke and others (1934), Chaudron (1921), Eastman and Evans (1924), Edmiston and Grace (1966), Schreiner and Grimes (1920), von Goldbeck (1949), Woehler and Balz (1921), and Woehler and Gunther (1923) were given zero weight.

Examination of Figure A.26 would indicate that there were two populations of data, one which the fitted curve passed through and another that is somewhat more oxidizing by about 0.2 log units. This author has no explanation for the observation.

Figures A.26 and A.27 and Table A.13 near here.

Cu_2O(cuprite) + Fe(s) = 2 Cu(s) + FeO(wus,sln)

Table A.14 contains a summary of the available data for this reaction. Figures A.28 and A.29 show the experimental data and the calculated enthalpies of reaction at 298.15 K as a function of the temperature of observation. As for other equilibria, the research of Kiukkola and Wagner (1957) show systematic drift and was given zero weight in the final evaluation. It must be noted that Kiukkola and Wagner (1957), in their pioneering work with solid electrolytes, used a sandwich-type technique. They made no provision that would block the oxygen gas coexisting with one buffer assemblage from bypassing the ceramic electrolyte and interfering with the response from the other buffer assemblage. As expected, the reported potentials were always less than the predicted potentials.

Figures A.28 and A.29 and Table A.14 near here.

NiO(bunsenite) + Fe(s) = Ni(s) + FeO(wus,sln)

Table A.15 contains a summary of the available data for this reaction. The experimental data for the potential difference between the nickel-bunsenite and the iron-wustite buffers are plotted on Figures A.30. The calculated enthalpies of reaction at 298.15 K are plotted on Figures A.31. The experimental range was from about 860 to 1620 K, which is almost the full temperature range for the stability of the iron-wustite coexistence.

The following studies were given zero weight based on the enthalpy-temperature plots: Asao and others (1970), Hoch and others (1962), Moriyama and others (1969), Pyun and M$\overset{a}{u}$ller(1969), Ramakrishnan and others (1975), Sjoeden and others (1986), Sreedharan and others (1977), and Trumm (1971). The thermochemical functions are consistent with O'Neill's (1987) study but the study became available after the optimization was completed.

Figures A.30 and A.31 and Table A.15 near here.

$3\ Fe(s) + 2\ O_2(g) = Fe_3O_4$(magnetite)

Figure A.32 contains the experimental equilibria for the formation of magnetite from the elements. The third law $\Delta_r H°(298)$ for each observation is plotted on Figure A.33. The data and the data from combustion calorimetry are summarized on Table A.16.

The early calorimetry by Mixter (1913) and by Roth and Weinert (1934) were given zero weight. The more recent studies by Humphrey and others (1952) and by Turnbull (1975) were used in the optimization. The agreement is good. The equilibrium studies by Barbi (1964a), Mallika and others (1986), Matsushit~~o~~a and Goto (1963), and Sugimoto and others (1980) were given zero weight. Electrochemical studies are unreliable in this temperature range because the electrolyte has a high resistance to oxygen ion conductivity at and below 873 K.

From activity measurements in Fe-S-O melts, Stofko and others (1974) calculated an equilibrium constant, log K, at 1473 K of 23.08 ± 0.10. The fitted value, 22.95, was in adequate agreement, but $\Delta_r H°(298)$ was -1120.4 kJ/mol.

Figures A.32 and A.33 and Table A.16 near here.

$0.25\ Fe_3O_4$(magnetite) + CO(g) = 0.75 Fe(s) + CO_2(g)

Marion (1955) determined the gas ratios needed to reverse the reaction. Refer to Figures A.34 and A.35 and Table A.17. However, while they are consistent with the data obtained for the reaction where the gases H_2 and H_2O were used, these data were given zero weight because the gas mixtures were metastable relative to the presence of solid carbon (graphite).

Figures A.34 and A.35 and Table A.17 near here.

$0.25\ Fe_3O_4$(magnetite) + H_2(g) = 0.75 Fe(s) + H_2O(g)

The experimental data for the reduction of magnetite with gas mixtures containing H_2 and H_2O are given on Figure A.36 and in summary on Table A.18. The corresponding enthalpies of reaction at 298.15 K for each of the experimental observations are given on Figure A.37. The experimental data by Chaudron (1921), by Fricke and others (1941), and by Woehler and Gunther (1923) were given zero weight because there was considerable scatter in the results. Again, as with the Ni-NiO data, the data by Rau (1972) below 720 K were given zero weight because they were shown to be unreliable at these lower temperatures. It should be noted, for this oxide pair they are consistent with the calculated equilibria whereas for the Ni-NiO data by Rau and Guedes de Carvalho (1973) there is considerable departure of the calculated data from the observed data.

Figures A.36 and A.37 and Table A.18 near here.

$2\ Fe_3O_4$(magnetite) = 6 FeO(wus,sln) + O_2(g)

The directly observed equilibria for the wustite-magnetite boundary are shown on Figure A.38 and in summary on Table A.19. The calculated enthalpy of reaction at 298.15 K for each observation is shown of Figures A.39 as a function of the temperature of observation. The research studies marked with an asterisk (*) on Table A.19 were used in this evaluation.

The fitted function is in poor agreement with the published data for this reaction. However, much of the published data were generated using unknown constants from the original experimental measurements. An example is the unavailable equilibrium data for the reaction CO(g) + 0.5 O_2(g) = CO_2(g) as used by Carel (1971) to convert the CO_2-CO ratios to log f(O_2). This emphasizes the need for authors to supply the original experimental data as well as any derived values. Fortunately, other data are available to constrain the fitting of the functions.

Studies that were given zero weight in the optimization were discarded because of the trends and scatter on the enthalpy-temperature plots. This author suspects that the observations by Rizzo (1968) represent a lack of equilibrium. It is possible that the wustite sample never came into chemical equilibrium with the magnetite during the run and the metastable equilibrium between magnetite and oxygen-rich wustite was observed.

Figures A.38 and A.39 and Table A.19 near here.

Fe_3O_4(magnetite) + Fe(s) = 4 FeO(wus,sln)

The measurement of the potential differences between the iron-wustite and the wustite-magnetite buffers are cited on Table A.20 and on Figure A.40. The above equation is the net for the two electrochemical cells. The calculated enthalpies of reaction at 298.15 K for each observation are given as a function of the temperature of the observation on Figure A.41. The data that are marked by an asterisk (*) on Table A.20 were used in the optimization. The calculated curve is in acceptable agreement with the experimental studies.

The study by Levitsky and others (1965) was kept in the optimization because the other data and the fitted function were consistent with the data and its precision. The data that were given zero weight had anomalous trends on the enthalpy-temperature plot.

Figures A.40 and A.41 and Table A.20 near here.

Fe_3O_4(magnetite) + CO(g) = 3 FeO(wus,sln) + CO_2(g)

Figure A.42 and Table A.21 summarize the experimental data for the reaction above. The data that were used are flagged with an asterisk (*). Figure A.43 supply plots of the enthalpies of reaction at 298.15 K as a function of the temperature of observation.

The fitted functions are in agreement with the observations cited here, unlike the data for the reaction between the gases CO_2 and CO and the solids iron and wustite where the calculated curve was bracketed by the study of Vallet and Raccah (1965) on one side and by the other studies on the other side. If there were a discrepancy in the calculated fugacity of oxygen for the given gas mixtures, the pattern would have been the same as for the earlier reaction.

Figures A.42 and A.43 and Table A.21 near here.

Fe_3O_4(magnetite) + H_2(g) = 3 FeO(wus,sln) + H_2O(g)

The experimental studies are cited on Table A.22 and plotted on Figure A.44. The calculated enthalpies of reaction at 298.15 K are plotted as a function of the temperature of observation on Figure A.45. The studies of Bulgakova and Zaitsev (1965), of Chaudron (1921), of Eastman and Evans (1924), of Woehler and Balz (1921) and of Woehler and Gunther (1923) were given zero weight. Most of the weight for this reaction was given to the research by Emmett and Shultz (1930, 1933) and by Rau (1972).

Figures A.44 and A.45 and Table A.22 near here.

Fe_3O_4(magnetite) + 2 Cu(s) = 3 FeO(wus,sln) + Cu_2O(cuprite)

The above is the net reaction for the potential difference between the wustite-magnetite assemblage and the copper-cuprite assemblage. The only available study for this reaction was the work of Kiukkola and Wagner (1957), but that study was given zero weight (Table A.23). The sandwich-type electrochemical cell was used by Kiukkola and Wagner (1957) in these early experiments. All electrochemical potentials reported in that study yielded unacceptable slopes or anomalously low potentials as shown on Figures A.46 and A.47.

Figures A.46 and A.47 and Table A.23 near here.

Fe_3O_4(magnetite) + Ni(s) = 3 FeO(wus,sln) + NiO(bunsenite)

The net reaction between the wustite-magnetite assemblage and the copper-cuprite assemblage is given by the above reaction. The available studies for this reaction are cited on Table A.24 and plotted on Figure A.48. The calculated enthalpies of reaction at 298.15 K are shown on Figure A.49 as a function of the temperature of observation. The research of Asao and others (1970) were given zero weight. Those data, as well as the associated potentials measured between wustite solid solutions and the nickel-bunsenite assemblage, have erroneous trends. The other research is in acceptable agreement.

Figures A.48 and A.49 and Table A.24 near here.

$2\ Fe(s) + 1.5\ O_2(g) = Fe_2O_3$(hematite)

Table A.25 gives the calorimetric enthalpies of formation of hematite from the elements. The data are erroneous and were given zero weight.

Table A.25 near here.

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2 Fe_3O_4(magnetite) + 0.5 O_2(g) = 3 Fe_2O_3(hematite)

The experimental data, outlined on Table A.26, are given graphically on Figures A.50. The calculated enthalpy of reaction for each of the experimental values is given on Figure A.51. Most of the enthalpies for the mass-spectrometry of Chizhikov and others (1971) plot outside of the coordinates and were given zero weight during the evaluation. The reported fugacities are too low. The research of Treadwell (1916) was given zero weight because an unreliable solid electrolyte was used. The work of Norton (1955), of Schwab and Kuestner (1981), and of Myers and Eugster (1983) are somewhat high. These studies were also given zero weight in the final analysis. Concerning the experiments of Myers and Eugster, research on other equilibria involving wustite are also high when compared with similar experiments by other workers. The experimental studies by Tretyakov and Khomyakov (1962), White and Richards (1949), and Schmahl and others (1969) have anomalous trends. These studies were given zero weight.

In evaluating the equilibria between magnetite and hematite, no correction was made for decreases in the activity of hematite due to solid solution. At 1651 K, the mole fraction of Fe_3O_4 in hematite is less than 0.014 and the mole fraction decreases with decreasing temperature (Greig and others, 1935). The activity of Fe_3O_4 in magnetite was calculated from the following formula (Salmon, 1961):

$$a(Fe_3O_4) = \frac{X_2}{0.25\ X_1 + X_2} \qquad \text{A.12}$$

where X_1 and X_2 are the mole fractions of Fe_2O_3 and Fe_3O_4 in the magnetite phase. The plot of the equilibrium constants against reciprocal temperature appear acceptable, however, the enthalpy plots appear to deviate above 1550 K. The adjustments in the activities may not be correct and should be examined with future research. Dieckmann (1982) has made a detailed study of the magnetite solid solution but it could not be included here because the experimental data were only presented on small graphs.

Based on the trend shown on the enthalpy-temperature plot, dropping the lower temperature experiments might be questioned. Consideration of data for electrochemical potential measurements against the Ni-NiO buffer and the Cu-Cu_2O buffer and reversals using H_2O-H_2 gas equilibria support the decision. These are discussed in the following subsections.

Figures A.50 and A.51 and Table A.26 near here.

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3 Fe_2O_3(hematite) + H_2(g) = 2 Fe_3O_4(magnetite) + H_2O(g)

Rau (1972) obtained reversals for the reaction. All data are summarized on Table A.27. These are plotted on Figure A.52. The calculated enthalpies of reaction at 298.15 K for the observations are given on Figure A.53. The fitted curve lies within only one of the three reversal brackets. However, the results are acceptable, considering the difficulties of maintaining a uniform mixture of H_2 and H_2O gases with such a difference in molecular weight.

The equilibrium constants reported for the above reaction by Woehler and Balz (1921) appear to be in error by a factor of 4. This correction was made during the data analysis.

The curvature on Figure A.52 appears to be anomalous. However, it must be noted that there are significant heat effects associated with the lambda anomalies in magnetite at 849.1 K ($10^3/T = 1.178$) and in hematite at 955.53 ($10^3/T = 1.047$). For more information, refer to the discussion in the section on heat capacity.

Figures A.52 and A.53 and Table A.27 near here.

$3\ Fe_2O_3$(hematite) + 2 Cu(s) = $2\ Fe_3O_4$(magnetite) + Cu_2O(cuprite)

The data for the comparison of the magnetite-hematite buffer with the copper-cuprite buffer are given on Figure A.54 and the calculated enthalpies of reaction at 298.15 K are given on Figure A.55. Table A.28 contains a summary of the available data for this reaction. Except for the research of Bonnet and Perrin (1978) which has a different slope, the studies are in good internal agreement and fit well by the mathematical model. These data and the results for the next reaction support the fitted functions for the thermochemistry for magnetite and hematite. The limited scatter of the data leaves little doubt as to what the activity of oxygen in equilibrium with magnetite and hematite should be.

Figures A.54 and A.55 and Table A.28 near here.

$3\ Fe_2O_3$(hematite) + Ni(s) = $2\ Fe_3O_4$(magnetite) + NiO(bunsenite)

The net reaction for the potential difference between the magnetite-hematite assemblage and the nickel-bunsenite assemblage is given by the reaction above. The experimental results are given on Figure A.56 and the calculated enthalpies of reaction at 298.15 K are given on Figure A.57. Table A.29 contains a summary of the available data for this reaction. The research of Moriyama and others (1969) were given zero weight because a sandwich-type technique was used.

The experiments at high pressures by Trumm (1981) and by Ulmer and others (1976) are not in agreement with each other. The fitted functions are in satisfactory agreement with the experiments by Trumm (1981). The data supplied by Ulmer and others (1976) were given zero weight in the optimization.

Figures A.56 and A.57 and Table A.29 near here.

$3\ Fe_2O_3$(hematite) + Fe(s) = 2 Fe_3O_4(magnetite) + FeO(wus,sln)

Blumenthal (1961) measured the potential difference between the iron-wustite and the magnetite-hematite buffers for oxygen by a stacked sandwich method (Figures A.58 and A.59). The pressed pellets for the buffers were separated by a sintered, CaO-doped zirconia disk. The vapor phase from the pellet on one side of the zirconia electrolyte could come in physical contact with the other pellet. It is believed that the observed decrease in the potential difference shown by this study was caused by the interference of the oxygen atmosphere on the magnetite-hematite pellet with the fugacity of oxygen for the iron-wustite pellet. The study was given zero weight.

The research by Gordeev and Tretyakov (1963) is also anomalous and was given zero weight. Jacobsson's (1985) research, which used a more sound electrochemical technique, is in good agreement with the other equilibria that were included in this study. The data above 1373 K were given zero weight because there are possible reactions with the zirconia electrolyte. All data are cited on Table A.30.

Figures A.58 and A.59 and Table A.30 near here.

The Polymorphic Reactions of Fe_2SiO_4(s1,s2,l)

The polymorphic phases are fayalite, the spinel structure, and the liquid. Table A.31 through A.33 gives the available data for the polymorphic reactions of the diferrous silicate. Figure A.60 shows the available experimental data and the inversion curves as calculated from the fitted functions. The correlation with the fitted curves and with the experimental enthalpies is satisfactory.

In optimizing the data for the melting of fayalite, 1490 K was taken as the congruent fusion temperature (Stebbins and Carmichael, 1984). Ohtani (1979) reported that fayalite and the spinel polymorph melted congruently at pressures above 50 kbars. In this optimization it was assumed that the incongruent melting curves as observed in the studies cited on Table A.32 were a reasonable approximation for the metastable congruent melting curve if the temperature at 1 bar was fixed at 1490 K. A reasonable fit of the phase equilibria was obtained. The invariant point (fayalite+spinel+liquid) was found to be 1810 K (1537°C) and 63.75 kbars. This result is in fair agreement with the value of 1520±25°C and 70±5 kbars reported by Ohtani (1979) but in excellent agreement with 1520° and 62 kbars as reported by Akimoto and others (1967).

Figure A.60 and Tables A.31, A.32, and A.33 near here.

$2\ Fe(s) + Si(s) + 2\ O_2(g) = Fe_2SiO_4$(fayalite)

King (1952) measured the enthalpy of formation of fayalite from the elements using a solution calorimeter (Table A.34). After correcting his data to be consistent with current data for solutions (Wagman and others, 1982), the revised value, -1479.7±1.9 kJ/mol, is in acceptable agreement with the fitted value of -1477.7±1.3 kJ/mol. Of the components in this study, the research relating to the properties of fayalite needs additional experiments. Lack of equilibrium is the major problem. This will be shown by some of the reactions to be discussed.

Table A.34 near here.

Fe_2SiO_4(fayalite) = 2 Fe(s) + SiO_2(quartz) + O_2(g)

The experimental data for these reactions are given on Table A.35 and Figure A.61 and the calculated enthalpies of reaction at 298.15 K are given on Figure A.62.

Interpretation of the experimental data is subject to question. Identification of the silica polymorphic groups (quartz, tridymite, or cristobalite) was not always made. The evaluator is left to use judgement as to phase assignment. Inversions among the polymorphic groups with increasing temperature are sluggish and achieving the stable equilibrium with decreasing temperature is non-existent. Within each polymorphic group, there are alpha-beta transitions that are rapid and reversible with some hysteresis. Myers and Eugster (1983) identified the starting material as being quartz but no explicit identification was made of the run products. Their data were interpreted as being in equilibrium with quartz, even though the temperatures of the run would be within the stability range of tridymite and cristobalite. Where identification was made in the remaining studies below, the polymorph was either cristobalite or tridymite plus cristobalite. All data other than those of Myers and Eugster (1983) were assumed to be in equilibrium with cristobalite.

The data of Myers and Eugster (1983) were given zero weight because the study, which contains data for several reactions at 1.01 bars, systematically departs from the available data for all reactions studied. The two reversed observations of Williams (1971) were given zero weight even though the reversal at 1541 K is consistent with the fitted curve. The observations of Nafziger and Muan (1967) were also given zero weight. Except for the reversal by Williams at 1451 K, the values deviate from the other data well beyond the reasonable precision in the data.

Schwab and Kuestner's (1981) data were used but the precision was lowered (increased in magnitude). All components of the study by Schwab and Kuestner (1981) have slightly higher oxygen potentials than comparable studies by other authors. The trend for this reaction is consistent with that observation. The fitted curve indicates that fayalite is slightly more stable than the experimental data would indicate.

Figures A.61 and A.62 and Table A.35 near here.

$0.5\ Fe_2SiO_4$(fayalite) + CO(g) = Fe(s) + $0.5\ SiO_2$(quartz) + CO_2(g)

The experimental data for the studies cited on Table A.36 are shown on Figure A.63 and the enthalpies of reaction at 298.15 K as a function of the temperature of observation are shown on Figure A.64. Agreement is reasonably good both among the studies and with the other data in the evaluation.

Figures A.63 and A.64 and Table A.36 near here.

$0.5\ Fe_2SiO_4(\text{fayalite}) + H_2(g) = Fe(s) + 0.5\ SiO_2(\text{quartz}) + H_2O(g)$

Berliner and Shapovlova (1966) reported data for the reduction of fayalite by hydrogen gas (Table A.37 and Figures A.65 and A.66). The data were not consistent with other studies and were given zero weight.

Figures A.65 and A.66 and Table A.37 near here.

$FeO(wus,sln) + 0.5\ Si_2O(quartz) = 0.5\ Fe_2SiO_4(fayalite)$

The above reaction is the net for the potential difference between the iron-wustite buffer and the quartz-fayalite-iron buffer. The studies are summarized on Table A.38 and shown on Figures A.67 and A.68. The research by Shiomi and others (1975) has an anomalous trend and was given zero weight. The study by O'Neill (1987) did not become available until after the completion of the evaluation. The study is consistent with the data by Levitsky and Ratiani (1970). However, both indicate fayalite is slightly less stable than the fitted thermochemistry.

Figures A.67 and A.68 and Table A.38 near here.

2 Fe(s) + SiO_2(quartz) + 2 Fe_3O_4(magnetite) = Fe_2SiO_4(fayalite) + 6 FeO(wus,sln)

The above reaction represents the net reaction for the potential difference between the quartz-fayalite-iron and the wustite-magnetite buffer assemblages. Eremenko and Filippov (1967) measured this potential difference and published an algebraic equation (Table A.39 and Figure A.69). However, their equation, as given, departs from the final function obtained in this research by over 40 kJ/mol. Their results were given zero weight in the final evaluation.

Figure A.69 and Table A.39 near here.

Fe_3O_4(magnetite) + 1.5 SiO_2(quartz) = 1.5 Fe_2SiO_4(fayalite) + 0.5 O_2(g)

Figure A.70 contains the data at one atmosphere that are cited in Table A.40. The corresponding enthalpies of reaction are given on Figure A.71.

All data were given zero weight in the final fitting of the model to the data. The data of Schwab and Kuestner (1981) did not approach equilibrium until the temperature exceeded 1200 K. The anomalously low fugacities of oxygen cannot be explained in any other way. Above 1200 K, the reported activities are somewhat higher than the calculated values from the fitted functions. This trend is consistent with the trend for other reactions reported by Schwab and Kuestner (1981). The data of Schwab and Sohnlein (1977) were given zero weight because the data scattered too much and also indicate lack of equilibrium. The data of Myers and Eugster (1983) were given zero weight because the experimental method produced higher activities of oxygen and systematic departure from the other available research for this and other reactions.

Figures A.70 and A.71 and Table A.40 near here.

Fe_3O_4(magnetite) + 1.5 SiO_2(quartz) + CO(g) = 1.5 Fe_2SiO_4(fayalite) + CO_2(g)

The two isolated observations for the reduction of magnetite and cristobalite to fayalite by CO(g) are shown on Figure A.72 and given on Table A.41. As indicated by the enthalpy-temperature plot (Figure A.73), the observation by Schwerdtfeger and Muan (1966), which has a low precision, is in acceptable agreement. However, the observation by Schenck and others (1932) was given zero weight in the final evaluation.

Figures A.72 and A.73 and Table A.41 near here.

Fe_3O_4(magnetite) + 1.5 SiO_2(quartz) + H_2(g) = 1.5 Fe_2SiO_4(fayalite) + H_2O(g)

The experimental data are cited on Table A.42. Because of the nature of the data, plots of the observed and calculated values could not be made. Figure A.74 is a plot of the enthalpy of reaction at 298.15 K against the temperature of observation. The data of Wones and Gilbert were believed to be measurements where equilibrium of the hydrogen gas was not attained on both sides of a platinum separator that was used as a permeable membrane for H_2. The balance of the data cited below were used in the final evaluation. For this reaction, Myers and Eugster (1983) used equipment similar to that used in the other citations for this reaction. The data, though scattered, are reasonably consistent with other work.

Figure A.74 and Table A.42 near here.

Fe_3O_4(magnetite) + 1.5 SiO_2(quartz) + 2 Cu(s) = 1.5 Fe_2SiO_4(fayalite) + Cu_2O(cuprite)

O'Neill (1987) measured the oxygen potential between the quartz-fayalite-magnetite buffer and the copper-cuprite buffer. These data became available after completion of the study. Refer to Table A.43 and Figures A.75 and A.76. They would place the quartz-fayalite-magnetite buffer at a lower activity of oxygen than found by this optimization. In order to accept O'Neill's data for the equilibria with fayalite, many other studies, believed to be correct, would be systematically in error. These studies include almost all studies relating to fayalite, to the combustion calorimetry by Mah and others (1967) and by Boyle and others (1954) on the oxides of copper and nickel, respectively, and most of the equilibria between bunsenite or cuprite and other phases.

Figures A.75 and A.76 and Table A.43 near here.

Fe_3O_4(magnetite) + 1.5 SiO_2(quartz) + Fe(s) = 1.5 Fe_2SiO_4(fayalite) + FeO(wus,sln)

The above equation is the net reaction for the potential difference between the quartz-fayalite-magnetite buffer and the iron-wustite buffer. Schwab and Sohnlein (1977) measured the potential differences between these buffers and obtained the scattered results shown on Table A.44 and Figures A.77 and A.78. The data were given zero weight in the evaluation.

Figures A.77 and A.78 and Table A.44 near here.

Summary

In this appendix, the results from analysis of 41 reactions and 3 polymorphic inversions in the seven-component chemical system Cu-Ni-Fe-Si-C-H-O were summarized. The data for these reactions were a major component of the optimization. For some reactions only a few observations were available; for others, many hundreds. For some reactions the observations were scattered and unuseable; for others they were highly correlated. Except for fayalite, which needs additional experimentation, and for wustite, which needs additional data at temperatures below 839 K or at higher pressures, the results of this optimization should stand without serious challenge.

APPENDIX B

FITTED CONSTANTS FOR THE MATHEMATICAL MODEL

In Chapter 5, a mathematical model for the common thermodynamic functions was supplied. The model and several additional empirical functions were used to fit the experimental data and to prepare the tables of properties given in Chapters 8 through 10. The functions and the fitted constants have many uses in addition to calculating the tabular data as was used here. Therefore, the constants are given in Table B.1. Tables B.2 and B.3 identify the equations into which the constants are to be inserted to calculate various properties. One caveat must be observed. For the use of these functions in the calculation of the properties of the wustite solid solution, the solution model being followed in any new application must be the same as the one used here.

In the actual optimization, the reference state was 1 atmosphere (=1.01325 bars). However, to comply with the recently adopted pressure convention of 1 bar, the constants in Table B.1 have been converted to the current reference pressure of 1 bar.

APPENDIX C

STANDARD DEVIATION FOR A PREDICTED "OBSERVABLE"

A predicted "observable" is any value calculated from the final set of refined constants and the equations given in Chapter 5. Therefore, all calculated thermodynamic properties given in Chapters 8 through 10 are predicted "observables".

The procedure for calculating the standard deviation, _sigma_, as given by Clifford (1973) was followed. The variance-covariance matrix, $\overline{M}$, was saved from the last refinement cycle to get the best fit for the mathematical model to the available data. The symmetrical, square matrix $\overline{M}$ contains the following elements:

$$(\overline{M}_x)_{ii} = [\mathrm{sigma}(x_i)]^2 \qquad \text{C.1}$$

$$(\overline{M}_x)_{ij} = \mathrm{rho}(x_i, x_j) \cdot \mathrm{sigma}(x_i) \cdot \mathrm{sigma}(x_j) \qquad \text{C.2}$$

where _ii_ represent the diagonal elements and _i_ and _j_ represent the elements off the diagonal of the matrix. The term sigma(x_i) is the variance of the _i_th fitted constant and the term rho(x_i,x_j) is the covariance between the _i_th and _j_th fitted constants in the fitting equation.

In matrix notation, the standard deviation of the predicted observable, sigma(y) is as follows:

$$\text{sigma}(y) = \sum_{i=1}^{n} \left[(\overline{M}_y)_{ii} \right]^{.5} \qquad \text{C.3}$$

where n is the number of fitted constants in the equation and

$$\overline{M}_y = (\overline{A}' \cdot \overline{M}_x \cdot \overline{A})^{-1} \qquad \text{C.4}$$

The elements of $\overline{A}$ are given by equation C.5 and

$\overline{A}'$ is the inverse of $\overline{A}$.

$$(\overline{A})_{ij} = \frac{\partial x_i}{\partial y_j} \qquad \text{C.5}$$

The partial derivative in equation C.5 is the derivative of the equation for the thermodynamic property with respect to each fitted constant, y_j.

For additional details, refer to Clifford (1973).

Recommended Standard Electrochemical Potentials and Fugacities of Oxygen for the Solid Buffers and Thermodynamic Data in the Systems Iron-Silicon-Oxygen, Nickel-Oxygen, and Copper-Oxygen

Part 2. Tables

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January 17, 1988

Recommended fugacities and standard electrochemical potentials for O_2 in the buffer pairs from 200 to 1800 K were derived from critical reviews of experimental data and thermodynamic theory. Included are C_p°, $H^\circ(T)-H^\circ(298)$, $[G^\circ(T)-H^\circ(298)]/T$, S°, $\Delta_f H^\circ$, $\Delta_f G^\circ$, V°, and the coefficients of volume expansion and of volume compression for the oxide phases.

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Table 2.1. Symbols and abbreviations used in this report.

Symbol	Description
$^{\circ}$	superscript designating that the property so noted is for the standard state of the phase at the temperature and standard state pressure.
A	Avogadro constant (=$6.0221367\cdot10^{23}$ mol^{-1})
a°	crystallographic cell edge for wustite (Angstroms).
a(T)	function in T giving the fugacity of oxygen at the iron-wustite boundary.
$a_{j,i}$	constants for the *j*th phase for use in algebraic equations for the thermodynamic functions.
log a( )	logarithm (base 10) of the activity of the chemical species contained within the parentheses.
b(T)	function in T giving the fugacity of oxygen at the wustite-magnetite boundary.
$b_{j,i}$	constants for the *j*th phase for use in algebraic equations for the volumetric functions.
C_P	heat capacity at constant pressure [J/(mol·K)].
C_{P_r}	heat capacity at a constant reference pressure, Pr [J/(mol·K)].
C°_{M}	magnetic component of the heat capacity at constant pressure [J/(mol·K)].
E	electrochemical potential (volts).
e(subscript)	property of an element.
e	base of natural (or Napierian) logarithms (= 2.7182818284·····).
F	the Faraday constant (= 96,485.309 coulombs/volt).

Table 2.1 Continued. Symbols and abbreviations used in this report.

Symbol	Description
f( )	fugacity of the chemical species contained within the parentheses (bars where 1 bar = 10^5 pascals).
g	Gibbs energy (J/mol) as defined in the mathematical model in Chapter 5.
G	Gibbs energy (J/mol).
$\Delta_f G^\circ$	Gibbs energy for formation from the elements (J/mol).
$\Delta_r G^\circ$	Gibbs energy of reaction (J/mol).
(g)	The physical state of the chemical species preceding the parentheses is gaseous.
h	enthalpy (J/mol) as defined in the mathematical model in Chapter 5.
H	enthalpy (J/mol).
$\Delta_f H^\circ$	isothermal enthalpy change for formation from the elements (J/mol).
$\Delta_r H^\circ$	isothermal enthalpy change for reaction (J/mol).
H(T)-H(Tr)	relative heat content (enth~~e~~alpy increment) of a phase between T and Tr (J/mol).
H(T)-H(298)	relative heat content (enth~~e~~alpy increment) of a phase between T and 298.15 K (J/mol).
i(subscript)	the *i*th phase of a series.
j(subscript)	the *j*th phase of a series.
j'_i	empirical exponential constant in the equation for the magnetic contribution to a thermodynamic property below the temperature of the lambda anomaly.

Table 2.1 Continued. Symbols and abbreviations used in this report.

Symbol	Description
j_i''	empirical exponential constant in the equation for the magnetic contribution to a thermodynamic property above the temperature of the lambda anomaly.
K	kelvin, the measure of absolute temperature.
log K	logarithm (base 10) of the equilibrium constant for a chemical reaction.
k	indexing constant in the series expansion of the equation for the magnetic contribution to a thermodynamic property.
k'	= 2 k - 1.
(l)	The physical state of the chemical species preceding the parentheses is liquid.
ln	natural (or Napierian) logarithm.
log	logarithm to the base 10.
n	stoichiometric coefficient in a chemical reaction.
n_e	number of electrons exchanged in an electrochemical cell.
N	mole fraction of a component.
P	pressure (bars where 1 bar = 10^5 pascals)
Pr	reference pressure (bars where 1 bar = 10^5 pascals)
r(T)	empirical function in absolute temperature for the temperature dependence of the intercept in the equation $\log f(O_2) = r(T) + s(T)\,x$. The term x is the amount of excess oxygen in the wustite formula FeO_{1+x}.
R	molar gas constant [= 8.314510 J/(mol·K)].

Table 2.1 Continued. Symbols and abbreviations used in this report.

Symbol	Description
s(T)	empirical function in absolute temperature for the temperature dependence of the slope in the equation $\log f(O_2) = r(T) + s(T)\,x$. The term x is the amount of excess oxygen in the wustite formula FeO_{1+x}.
S	entropy [J/(mol·K)].
S°(0)	entropy of a phase at the absolute zero of temperature.
(s)	The physical state of the chemical species preceding the parentheses is solid.
T	temperature (K).
Tr	reference temperature (K).
T_C	critical temperature; the temperature of the maximum for a lambda anomaly (K).
T_N	critical temperature for a Neel-type magnetic transition.
V	molar volume (cm^3/mol).
Vr	molar volume at a reference point in temperature and pressure (cm^3/mol).
w	weight factor in regression analysis; = 1/($precision^2$).
x	moles of excess oxygen in wustite, FeO_{1+x}.
x_a	moles of excess oxygen in wustite, FeO_{1+x}, coexisting with metallic iron.
x_b	moles of excess oxygen in wustite, FeO_{1+x}, coexisting with magnetite.
y	moles of iron deficiency in wustite, $Fe_{1-y}O$.
z	moles of iron deficiency in magnetite, $Fe_{3-z}O_4$.

Table 2.1 Continued. Symbols and abbreviations used in this report.

Symbol	Description
alpha	coefficient of volume expansion (K^{-1}).
beta	coefficient of volume compression (bar^{-1}).
θ_D	Debye characteristic temperature (kelvin).
tau	ratio of the absolute temperature to the temperature T_C of a critical phenomenon (= T/T_C).

Table 2.2 Critical constants and conversion units.

Atomic Weights

Source: IUPAC (Inorganic Chemistry Division) Commission on Atomic Weights and Isotopic Abundances, (1986)

Name	Symbol	Value and Units
Carbon	C	12.011 g/mol
Copper	Cu	63.546 g/mol
Iron	Fe	55.847 g/mol
Hydrogen	H	1.00794 g/mol
Nickel	Ni	58.69 g/mol
Oxygen	O	15.9994 g/mol
Silicon	Si	28.0855 g/mol

Fundamental Constants

Source: Cohen and Taylor (1986). The digits in parentheses are the one-standard-deviation uncertainty in the last digits of the given value.

Avogadro constant	A	$6.0221367(36)\cdot10^{23}$ mol^{-1}
Faraday	F	96,485.309(29) J/(V·mol)
Molar gas constant	R	8.314510(70) J/(mol·K)

Defined Units

Standard atmosphere	atm	101.325 kPa (exact)
Bar	b	100.000 kPa (exact)
Thermochemical calorie	cal	4.184 J (exact)

Table 2.2 Critical constants and conversion units.

Conversion Factors From Non-SI Units to SI Units

0°C = 273.15 K (exact)

1 Å = 10^{-10} m

1 cm = 10^{-2}m

1 bar = 100,000 Pa (exact)

1 atm = 101,325 Pa (exact)

1 cal = 4.184 J (exact)

1 g/cm^3 = 1,000 kg/m^3

Table 7.01. Primary data used in the fitting of the equation for volume of nickel crystal and liquid, Ni. Sources flagged with an asterisk (*) were used in the optimization.

Source	Range T(K)	 P(kb)	Number of Obs.	Data Type
* Birch (1966)	293	0.001-30	6	(V-Vr)/Vr
* Fraser and Hallett (1961)	150-300	0.001	4	alpha
* Nix and MacNair (1941)	150-761	0.001	181	(V-Vr)/Vr
* Owen and Yates (1936)	285-881	0.001	42	V
Robie and others (1978)	298	0.001	1	V
* Saito and others (1969a,b)	1723-2423	0.001	15	V

Table 7.02. Primary data used in the fitting of the equation for volume of bunsenite, NiO. Sources flagged with an asterisk (*) were used in the optimization.

Source	Range T(K)	Range P(kb)	Number of Obs.	Data Type
* Barrett and Evans (1964)	293	0.001	1	V
Bickelhaupt and others (1967)	293-1476	0.001	14	V
* Clende~~n~~nen and Drickamer (1966)	298	0.001-275	8	V
* Gillam and Holden (1963)	532-1573	0.001	6	V
* Leipold and Nielssen (1964)	293-2023	0.001	10	V-Vr
* Melik-Davtyan and others (1966)	73-1179	0.001	33	V-Vr
* Rooksby (1948)	90-548	0.001	3	V
* Srivastava and others (1977)	105-813	0.001	8	V
* Wakabayashi and others (1968)	293	0.001-80	9	V
Wisely (1962)	298-1073	0.001	8	V-Vr

Table 7.03. Primary data used in the fitting of the equation for volume of iron, Fe. Sources flagged with an asterisk (*) were used in the optimization.

Source	Range T(K)	 P(kb)	Number of Obs.	Data Type
		alpha iron		
* Basinski and others (1955)	293-1189	0.001	17	V
	1662-1807	0.001	5	V
Birch (1966)	298	0.001-30	6	V
Clende~~n~~nen and Drickamer (1964)	298	0.001-300	6	V-Vr
Esser and Muller (1933)	293-1153	0.001	61	V/Vr
* Fraser and Hallett (1961)	150-300	0.001	4	alpha
* Giles and others (1971)	300	0.001-163	25	V
* Jephcoat and others (1986)	298	0.001	1	V
	298	0.001-164	7	V-Vr
* Mao and Bell (1979)	298	0.001	1	V
* Nix and MacNair (1941)	152-958	0.001	150	(V-Vr)/Vr
Robie and others (1978)	298	0.001	1	V
Skinner (1966)	273-873	0.001	4	V
* Takahashi and others (1968)	296	0.001-152	8	V
* Watanabe and others (1981)	673-1184	0.001	12	V
	1673-1809	0.001	4	V
* Wilburn and Bassett (1978)	298	0.001-108	13	V-Vr
		Gamma Iron		
* Basinski and others (1955)	1189-1661	0.001	9	V
Esser and Muller (1933)	1173-1373	0.001	14	V/Vr
* Gorton and others (1965)	1193-1343	0.001	4	V
* Newkirk (1957)	298	0.001	1	V
* Watanabe and others (1981)	1184-1673	0.001	11	V

Table 7.04. Primary data used in the fitting of the equation for volume of wustite, $Fe_{1-y}O$. Sources flagged with an asterisk (*) were used in the optimization.

Source	T(K)	Range P(kb)	Comp(="y")	Number of Obs.	Data Type
* Akimoto (1972)	298	0.001	0.000	1	V
Arkhanov and Kuznetsov (1966)	293-723	0.001	?	2	(V-Vr)/Vr
* Bonczar and Graham (1982)	293	0.001	0.061	1	V
* Carel and Gavarri (1976)	293	0.001	0.087-0.094	30	V
	293	0.001	0.042-0.107	42	V
* Carter (1959)	373-1273	0.001	?	5	(V-Vr)/Vr
Clendennen and Drickamer (1966)	293	0.001-276	0.067	9	V
* Fujii and Meussner (1968)	298	0.001	0.000-0.121	3	V
* Gorton (1965)	873-1273	0.001	0.076	5	V
Hayakawa and others (1972)	1184-1450	0.001	0.121-0.126	36	V
	1223-1323	0.001	0.045-0.123	64	V
* Hazen (1981)	298	0.001	0.053	1	V
	298	6-167	0.053	1	V/Vr
	298	0.001	0.070	1	V
	298	6-55	0.070	1	V/Vr
	298	0.001	0.100	1	V
	298	6-55	0.100	1	V/Vr
* Hentschel (1970)	293	0.001	0.000	2	V
* Jackson and others (1985)	293	0.001	?	1	beta
Jeanloz and Sato-Sorenson (1986)	298	0.001	0.055	22	V
* Levin and Wagner (1966)	293	0.001	0.046-0.115	17	V
* Mao and others (1969)	293	0.001-256	0.099	4	V
* Marion (1955)	293	0.001	0.054-0.122	13	V
Robie and others (1978)	298	0.001	0.053	1	V
* Touzelin (1974)	1073-1348	0.001	0.044-0.126	61	V
	298,503	0.001	0.000	2	V
* Will and others (1980)	293	0.001-196	0.059	36	V
* Yagi and others (1985)	298	0.001-142	0.020	8	V

Table 7.05. Experimentally observed Neel temperatures (K) for wustite, $Fe_{1-y}O$, as a function of the iron content. Koch and Fine (1967) and Michel and others (1970) derived the temperatures from measurements of magnetic suscept~~a~~iblility. Mainard and others (1968) and Todd and Bonnickson (1951) derived the temperatures from calorimetry. The temperatures in parentheses are data measured by Koch and Fine (1967) but readjusted by Mainard and others (1968).

1-y (moles)	Koch and Fine (1967)	Mainard and others (1968)	Michel and others (1970)	Todd and Bonnickson (1951)
1.000	-	-	198	-
0.947	-	-	-	188.5
0.944	-	179	190.5	-
0.937	-	187	192	-
0.934	-	-	191	-
0.932	199	(175)	-	-
0.937	-	189	-	-
0.923	-	190	-	-
0.921	-	-	190	-
0.917	-	-	190.5	-
0.905	-	-	193	-
0.899	-	197	-	-
0.898	-	-	193	-
0.896	209	(189)	-	-
0.892	-	-	194.5	-

Table 7.06. Primary data used in the fitting of the equation for volume of hematite, Fe_2O_3. Sources flagged with an asterisk (*) were used in the optimization.

Source	Range		Number of Obs.	Data Type
	T(K)	P(kb)		
* Falzone and Stacey (1982)	353	0.001	1	alpha
* Finger and Hazen (1980)	298	0.001-52	6	V-Vr
* Finger and Hazen (1980)	298	0.001	1	V
* Gorton and others (1965)	298-1273	0.001	6	V
Lewis and Drickamer (1966)	298	0.001-230	9	V-Vr
Lewis and Drickamer (1966)	298	0.001	1	V
* Neskovic (1984)	152-1225	0.001	32	V
* Rigby and others (1945)	373-1473	0.001	11	(V-Vr)/Vr
Robie and others (1978)	298	0.001	1	V
* Sato and Akimoto (1979)	298	0.001-111	15	V-Vr
* Wilburn and others (1978)	293	0.001-115	36	V-Vr
Willis and Rooksby (1952)	293-1023	0.001	2	V

Table 7.07. Primary data used in the fitting of the equation for volume of fayalite, Fe_2SiO_4. Sources flagged with an asterisk (*) were used in the optimization.

Source	Range T(K)	Range P(kb)	Number of Obs.	Data Type
* Hazen (1977)	77-296	0.001	3	V
* Hazen (1977)	296	0.001-42	3	V
* Kudoh and Takeda (1986)	298	0.001-140	6	V
* Rigby and others (1945)	373-1273	0.001	9	(V-Vr)/Vr
Schwab and Sohnlein (1977)	298	0.001	2	V
* Smyth (1975)	293-1173	0.001	6	V
Suwa (1964)	293-1073	0.001	17	(V-Vr)/Vr
* Suzuki and others (1981)	223-1273	0.001	22	V-Vr
* Takei (1978)	293-400	0.001	2	V
* Yagi and others (1974)	296	0.001-73	22	V/Vr

Table 7.08. Primary data used in the fitting of the equation for volume of diferrous silicate (spinel structure), Fe_2SiO_4. Sources flagged with an asterisk (*) were used in the optimization.

Source	Range T(K)	Range P(kb)	Number of Obs.	Data Type
* Mao and others (1969)	298	0.001	1	V
* Mao and others (1969)	281-669	0.001	8	(V-Vr)/Vr
* Mao and others (1969)	298	0.001-255	12	V/Vr
Marumo and others (1977)	298	0.001	1	V
* Sato (1977)	298	0.001-78	8	V/Vr
* Wilburn and Bassett (1978)	298	0.001-154	9	V/Vr
* Yamanaka (1986)	293-973	0.001	5	V

Table 7.09. Primary data used in the fitting of the equation for volume of magnetite, Fe_3O_4. Sources flagged with an asterisk (*) were used in the optimization.

Source	Range T(K)	P(kb)	Number of Obs.	Data Type
Arkharov and Bogoslovsky (1972)	673-1373	0.001	3	(V-Vr)/Vr
* Ellefson and Taylor (1934)	104-299	0.001	4	V
* Finger and others (1986)	298	0.001-45	5	V/Vr
Finger and others (1986)	298	0.001	1	V
* Gorton and others (1965)	298-1273	0.001	15	V
* Mao and others (1974)	296	0.001-320	13	V
* Nakagiri and others (1986)	298	0.001-44	36	V/Vr
* Nakagiri and others (1986)	298	0.001	1	V
* Nakagiri and others (1985)	293	0.001	3	beta
Sharma (1950)	293-985	0.001	39	(V-Vr)/Vr
* Tombs and Rooksby (1951)	165-298	0.001	2	V
* Wilburn and Bassett (1977)	293	0.001-65	10	V
* Yoshida and Iida (1977, 1979)	122-295	0.001	4	V

Table 7.10. Primary data used in the fitting of the thermal equations for tenorite, CuO. Sources flagged with an asterisk (*) were used in the optimization.

Source	Range T (K)	Number of Obs.	Observation	Error Percent
Clusius and Harteck (1928)	110-200	10	Cp	+0.4±6.0
* Hu and Johnson (1953)	146-297	33	Cp	+0.0±0.4
* Mah and others (1967)	298-1400	17	H(T)-H(298)	-0.1±0.2
Millar (1929)	130-301	54	Cp	+0.6±1.2

Table 7.11. Primary data used in the fitting of the thermal equations for cuprite and the dicuprous oxide liquid, $Cu_2O(s,l)$. Sources flagged with an asterisk (*) were used in the optimization.

Source	Range T (K)	Number of Obs.	Observation	Error Percent
Hu and Johnson (1951)	203-299	13	Cp	+1.2±0.4
* Mah and others (1967)	156-297	15	Cp	+0.0±0.1
* Mah and others (1967)	298-1509	20	H(T)-H(298)	-0.2±0.3
* Mah and others (1967)	1520-1600	4	H(T)-H(298)	+0.0±0.1
Millar (1929)	125-291	15	Cp	-0.6±0.9

Table 7.12. Primary data used in the fitting of the thermal equations for bunsenite, NiO. Sources flagged with an asterisk (*) were used in the optimization.

Source	Range T (K)	Number of Obs.	Observation	Error Percent
* Hemingway (1984)	338-846	136	Cp	+0.1±0.7
* King (1957)	206-295	10	Cp	-0.3±0.5
* King and Christensen (1958)	298-1810	24	H(T)-H(298)	-2.0±0.5
* Seltz and others (1940)	204-296	9	Cp	+0.7±1.0
* Tomlinson and others (1955)	273-1108	31	H(T)-H(298)	-0.4±0.4

Table 7.13. Primary data used in the fitting of the thermal equations for wustite, $Fe_{1-y}O$. Sources flagged with an asterisk (*) were used in the optimization.

Source	Range T (K)	Number of Obs.	Observation	Error Percent
* Coughlin and others (1951)	298-1614	25	H(T)-H(298)	0.0±0.8
Millar (1929)	103-301	38	Cp	+5.2±3.0
Rogez and others (1982)	1179	6	H(T)-H(300)	-4.9
* Todd and Bonnickson (1951)	104-297	31	Cp	0.0±1.1
Vladimirov and Ponomarev (1959)	273-1373	eqn	Cp	+6.0±1.0

Table 7.14. Primary data used in the fitting of the thermal equations for hematite, Fe_2O_3. Sources flagged with an asterisk (*) were used in the optimization.

Source	Range T (K)	Number of Obs.	Observation	Error Percent
* Coughlin and others (1951)	298-1757	31	H(T)-H(298)	0.0±0.7
Esser and others (1933)	273-1073	7	H(T)-H(273)	-5.0±6.6
* Grønvold and Samuelsen (1975)	302-1055	79	Cp	0.0±1.0
* Grønvold and Westrum (1959)	150-354	25	Cp	-0.2±0.5
* Krupka (1974)	340-720	21	Cp	-0.5±0.6
Parks and Kelley (1926)	187-289	13	Cp	+1.2±1.2
Reznitsky and Filippova (1972)	300-1000	7	H(T)-H(298)	????????
Roth and Bertram (1929)	293-1097	8	H(T)-H(293)	-1.4±1.0

Table 7.15. Primary data used in the fitting of the thermal equations for fayalite and the diferrous liquid, Fe_2SiO_4(sl,l). Sources flagged with an asterisk (*) were used in the optimization.

Source	Range T (K)	Number of Obs.	Observation	Error Percent
* Kelley (1941)	154-295	15	Cp	+0.4±0.3
* Orr (1953)	298-1370	13	H(T)-H(298)	-0.3±0.6
* Orr (1953)	1578-1733	5	H(T)-H(298)	0.0±0.2
Osako (1980)	280-420	8	Cp	-0.5±4.4
* Robie and others (1982)	154-381	40	Cp	0.0±0.2
Roth and Bertram (1929)	293-1161	6	H(T)-H(298)	+4.8±7.5
* Stebbins and Carmichael (1984)	1490	1	mH°	0.0
* Watanabe (1982)	350-700	18	Cp	-0.4±0.9

Table 7.16. Primary data used in the fitting of the thermal equations for diferrous silicate (spinel structure), $Fe_2SiO_4(s2)$. Sources flagged with an asterisk (*) were used in the optimization.

Source	Range T (K)	Number of Obs.	Observation	Error Percent
* Agoshkov (1985)	240-1170	16	H(T)-H(273)	+1.1±0.6
Osako (1980)	280-420	8	Cp	-0.3±4.0
* Watanabe (1982)	350-700	15	Cp	-0.6±0.6

Table 7.17. Primary data used in the fitting of the thermal equations for magnetite, Fe_3O_4. Sources flagged with an asterisk (*) were used in the optimization.

Source	Range T (K)	Number of Obs.	Observation	Error Percent
* Bartel and Westrum (1975)	304-548	34	Cp	+0.3±0.2
* Coughlin and others (1951)	298-1825	29	H(T)-H(298)	-0.4±0.7
Esser and others (1933)	273-1273	9	H(T)-H(273)	-8.4±2.0
* Gronvold and Sveen (1974)	300-1044	99	Cp	+1.0±1.3
Millar (1929)	153-300	12	Cp	-0.9±2.0
Parks and Kelley (1926)	153-295	7	Cp	+1.4±0.4
Roth and Bertram (1929)	293-1056	7	H(T)-H(293)	-1.0±1.5
* Westrum and Gronvold (1969)	159-348	22	Cp	+0.1±0.5

Table 7.18. Entropies, S°(T), for the oxides and the diferrous silicates as derived from the optimization of the experimental data and the values for S°(T)-S°(0) calculated from integration of calorimetric data.

Phase	This Study S°(298) J/(mol K)	Other Research S°(298)-S°(0) J/(mol K)	Other Research Source
Tenorite, CuO	42.60±0.09	42.63±0.08	Hu and Johnson (1953)
Cuprite, Cu_2O	92.37±0.09	92.38±0.40	Mah and others (1967)
		93.14±2.1	Gregor (1962), Hu and Johnson (1951)
Bunsenite, NiO	36.70±0.33	37.99±0.16	King (1957)
FeO	63.46±0.71	----	----
Wustite, $Fe_{1-y}O$	57.61	57.49±0.10	Todd and Bonnickson (1951)
Hematite, Fe_2O_3	87.48±0.06	87.40±0.09	Grønvold and Westrum (1959)
Fayalite, Fe_2SiO_4	150.95±1.01	151.00±0.20	Robie and others (1982)
(*Spinel*), Fe_2SiO_4	139.63±3.6	----	----
Magnetite, Fe_3O_4	145.44±0.32	146.15±0.15	Westrum and Grønvold (1969)

Table 7.19. Summary of data for tenorite by reaction. The second column shows the weighted results from this study. The third column gives the average of the third-law $\Delta_r H°(298)$ data for each reaction. The last column gives the $\Delta_f H°(298)$ for tenorite calculated from the averages. The last calculation assumes that all other data are correct. Compare these values with the last entry which was derived from this study.

Reaction	$\Delta_r H°(298)$ (kJ/mol)		$\Delta_f H°(298)$ (kJ/mol)
	This Study	Average for Reaction	Calculated from Average
$2\ Cu + O_2 = 2\ CuO$	-311.320±0.418	-311.540	-155.770
$Cu_2O + 0.5\ O_2 = 2\ CuO$	-140.688±0.442	-140.778	-155.705
$2\ CuO + Ni = Cu_2O + NiO$	-99.589±0.573	-99.348	-155.780
Enthalpy of formation, $\Delta_f H°(298)$, from weighted, least-squares optimization			-155.660 ±0.209

Table 7.20. Summary of data for cuprite by reaction. The second column shows the weighted results from this study. The third column gives the average of the third-law $\Delta_r H°(298)$ data for each reaction. The last column gives the $\Delta_f H°(298)$ for cuprite calculated from the averages. The last calculation assumes that all other data are correct. Compare these values with the last entry which was derived from this study.

Reaction	$\Delta_r H°(298)$ (kJ/mol) This Study	$\Delta_r H°(298)$ (kJ/mol) Average for Reaction	$\Delta_f H°(298)$ (kJ/mol) Calculated from Average
$2\ Cu + 0.5\ O_2 = Cu_2O$	-170.631±0.226	-170.689	-170.689
$Cu_2O + CO = 2\ Cu + CO_2$	-112.350±0.226	-----	-----
$Cu_2O + 0.5\ O_2 = 2\ CuO$	-140.688±0.442	-140.778	-170.541
$Cu_2O + Fe = 2\ Cu + FeO$	-91.501±0.469	-91.263	-170.869
$3\ Fe_2O_3 + 2\ Cu = 2\ Fe_3O_4 + Cu_2O$	70.875±0.728	70.601	-170.905
$Fe_3O_4 + 1.5\ SiO_2 + 2\ Cu = 1.5\ Fe_2SiO_4(sl) + Cu_2O$	-95.462±2.016	-----	-----
$Fe_3O_4 + 2\ Cu = 3\ FeO + Cu_2O$	159.612±1.277	-----	-----
$Cu_2O + Ni = 2\ Cu + NiO$	-69.646±0.410	-69.733	-170.544
$2\ CuO + Ni = Cu_2O + NiO$	-99.589±0.573	-99.348	-170.390
Enthalpy of formation, $\Delta_f H°(298)$, from weighted, least-squares optimization			-170.631 ±0.226

Table 7.21. Summary of data for bunsenite by reaction. The second column shows the weighted results from this study. The third column gives the average of the third-law $\Delta_r H^\circ(298)$ data for each reaction. The last column gives the $\Delta_f H^\circ(298)$ for bunsenite calculated from the averages. The last calculation assumes that all other data are correct. Compare these values with the last entry which was derived from this study.

Reaction	$\Delta_r H^\circ(298)$ (kJ/mol)		$\Delta_f H^\circ(298)$ (kJ/mol)
	This Study	Average for Reaction	Calculated from Average
$Ni + 0.5\ O_2 = NiO$	-240.277±0.374	-239.939	-239.939
$NiO + CO = Ni + CO_2$	-42.703±0.374	-42.778	-240.192
$NiO + H_2 = Ni + H_2O(g)$	-1.549±0.374	-1.715	-240.111
$Cu_2O + Ni = 2\ Cu + NiO$	-69.646±0.410	-69.733	-240.364
$2\ CuO + Ni = Cu_2O + NiO$	-99.589±0.573	-99.348	-240.036
$NiO + Fe = Ni + FeO$	-21.855±0.554	-21.790	-240.342
$Fe_3O_4 + Ni = 3\ FeO + NiO$	89.965±1.312	89.480	-240.762
$3\ Fe_2O_3 + Ni = 2\ Fe_3O_4 + NiO$	1.229±0.790	1.058	-240.448
Enthalpy of formation, $\Delta_f H^\circ(298)$, from weighted, least-squares optimization			-240.277 ±0.374

Table 7.22. Summary of data for ferrous oxide by reaction. The second column shows the weighted results from this study. The third column gives the average of the third-law $\Delta_r H°(298)$ data for each reaction. The last column gives the $\Delta_f H°(298)$ for ferrous oxide calculated from the averages. The last calculation assumes that all other data are correct. Compare these values with the last entry which was derived from this study.

	$\Delta_r H°(298)$ (kJ/mol)		$\Delta_f H°(298)$ (kJ/mol)
Reaction	This Study	Average for Reaction	Calculated from Average
2 FeO = 2 Fe + O_2	524.266±0.822	524.547	-262.273
2 FeO = 2 Fe + O_2	524.266±0.822	523.687	-261.843
FeO + CO = Fe + CO_2	-20.848±0.411	-20.427	-262.558
FeO + H_2 = Fe + H_2O(g)	20.306±0.411	20.634	-262.461
Cu_2O + Fe = 2 Cu + FeO	-91.501±0.469	-91.263	-261.895
NiO + Fe = Ni + FeO	-21.855±0.554	-21.790	-262.068
3 Fe_2O_3 + Fe = 2 Fe_3O_4 + FeO	-20.626±0.972	-20.684	-262.191
FeO + 0.5 SiO_2 = 0.5 Fe_2SiO_4(sl)	-21.383±0.780	-21.072	-262.444
2 Fe_3O_4 + 3 SiO_2 + 2 Fe = 3 Fe_2SiO_4(sl) + 2 FeO	8.168±4.328	-----	-----
2 Fe_3O_4 = 6 FeO + O_2	660.458±2.511	660.318	-262.156
Fe_3O_4 + CO = 3 FeO + CO_2	47.262±1.256	47.489	-262.057

Table 7.22. Summary of data for ferrous oxide by reaction. Continued.

Reaction	$_rH°(298)$ (kJ/mol) This Study	$_rH°(298)$ (kJ/mol) Average for Reaction	$_fH°(298)$ (kJ/mol) Calculated from Average
$Fe_3O_4 + H_2 = 3\ FeO + H_2O(g)$	88.416±1.256	88.822	-261.998
$Fe_3O_4 + 2\ Cu = 3\ FeO + Cu_2O$	159.612±1.277	-----	-----
$Fe_3O_4 + Ni = 3\ FeO + NiO$	89.965±1.312	89.480	-262.294
$2\ Fe + SiO_2 + 2\ Fe_3O_4 = Fe_2SiO_4(sl) + 6\ FeO$	93.545±2.839	-----	-----
$Fe_3O_4 + Fe = 4\ FeO$	68.110±1.661	67.943	-262.174
Enthalpy of formation, $\Delta_fH°(298)$, from weighted, least-squares optimization			-262.133 ~~±0.411~~ ±0.923

Table 7.23. Summary of data for hematite by reaction. The second column shows the weighted results from this study. The third column gives the average of the third-law $\Delta_r H°(298)$ data for each reaction. The last column gives the $\Delta_f H°(298)$ for hematite calculated from the averages. The last calculation assumes that all other data are correct. Compare these values with the last entry which was derived from this study.

Reaction	$\Delta_r H°(298)$ (kJ/mol) This Study	$\Delta_r H°(298)$ (kJ/mol) Average for Reaction	$\Delta_f H°(298)$ (kJ/mol) Calculated from Average
2 Fe + 1.5 O_2 = Fe_2O_3	-824.928±0.149	-----	-----
3 Fe_2O_3 + H_2 = 2 Fe_3O_4 + H_2O(g)	-0.320±0.705	-1.485	-824.539
2 Fe_3O_4 + 0.5 O_2 = 3 Fe_2O_3	-241.506±0.705	-241.694	-824.991
3 Fe_2O_3 + Fe = 2 Fe_3O_4 + FeO	-20.626±0.972	-20.684	-824.908
3 Fe_2O_3 + 2 Cu = 2 Fe_3O_4 + Cu_2O	70.875±0.728	70.601	-824.836
3 Fe_2O_3 + Ni = 2 Fe_3O_4 + NiO	1.229±0.790	1.058	-824.871
Enthalpy of formation, $\Delta_f H°(298)$, from weighted, least-squares optimization			-824.928 ~~±0.149~~ ±3.158

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Table 7.24. Summary of data for fayalite (=s1) by reaction. Except as noted for the melting of fayalite, the second column shows the weighted results from this study. The third column gives the average of the third-law $\Delta_r H°(298)$ data for each reaction. The last column gives the $\Delta_f H°(298)$ for fayalite (=s1) calculated from the averages. The last calculation assumes that all other data are correct. Compare these values with the last entry which was derived from this study.

Reaction	$\Delta_r H°(298)$ (kJ/mol) This Study	$\Delta_r H°(298)$ (kJ/mol) Average for Reaction	$\Delta_f H°(298)$ (kJ/mol) Calculated from Average
$Fe_2SiO_4(s1) = Fe_2SiO_4(s2)$	6.767±3.064	6.623	-1477.589
$Fe_2SiO_4(s1) = Fe_2SiO_4(l)$ ($_m H°(1490)$=	88.049±2.315	88.709	-1478.393)
$2\ Fe + Si + 2\ O_2 = Fe_2SiO_4(s1)$	-1477.733±1.324	-1479.706	-1479.706
$Fe_2SiO_4(s1) = 2\ Fe + SiO_2 + O_2$	567.031±1.324	563.678	-1474.380
$0.5\ Fe_2SiO_4(s1) + CO = Fe + 0.5\ SiO_2 + CO_2$	0.535±0.662	0.792	-1478.247
$0.5\ Fe_2SiO_4(s1) + H_2 = Fe + 0.5\ SiO_2 + H_2O(g)$	41.689±0.662	-----	-----
$FeO + 0.5\ SiO_2 = 0.5\ Fe_2SiO_4(s1)$	-21.383±0.780	-21.072	-1477.111
$2\ Fe_3O_4 + 3\ SiO_2 = 3\ Fe_2SiO_4(s1) + O_2$	532.187±4.000	-----	-----
$Fe_3O_4 + 1.5\ SiO_2 + CO = 1.5\ Fe_2SiO_4(s1) + CO_2$	-16.887±2.000	-14.667	-1476.253
$Fe_3O_4 + 1.5\ SiO_2 + H_2 = 1.5\ Fe_2SiO_4(s1) + H_2O(g)$	24.273±2.000	23.456	-1478.266
$Fe_3O_4 + 1.5\ SiO_2 + 2\ Cu = 1.5\ Fe_2SiO_4(s1) + Cu_2O$	-95.462±2.016	-----	-----

Table 7.24. Summary of data for fayalite (=sl) by reaction. Continued.

Reaction	${}_rH^\circ(298)$ (kJ/mol) This Study	${}_rH^\circ(298)$ (kJ/mol) Average for Reaction	${}_fH^\circ(298)$ (kJ/mol) Calculated from Average
$Fe_3O_4 + 1.5\ SiO_2 + Fe = 1.5\ Fe_2SiO_4(sl) + FeO$	3.906±2.044	-----	-----
$2\ Fe + SiO_2 + 2\ Fe_3O_4 = Fe_2SiO_4(sl) + 6\ FeO$	93.545±2.839	-----	-----
Enthalpy of formation, $\Delta_fH^\circ(298)$, from weighted, least-squares optimization			-1477.733 ±1.324

Table 7.25. Summary of data for the diferrous silicate (spinel structure, =s2) by reaction. Except as noted for the melting of the spinel phase, the second column shows the weighted results from this study. The third column gives the average of the third-law $\Delta_r H^\circ(298)$ data for each reaction. The last column gives the $\Delta_f H^\circ(298)$ for the diferrous silicate (spinel structure, =s2) calculated from the averages. The last calculation assumes that all other data are correct. Compare these values with the last entry which was derived from this study.

Reaction		$\Delta_r H^\circ(298)$ (kJ/mol) This Study	$\Delta_r H^\circ(298)$ (kJ/mol) Average for Reaction	$\Delta_f H^\circ(298)$ (kJ/mol) Calculated from Average
$Fe_2SiO_4(s1) = Fe_2SiO_4(s2)$		6.767±3.064	6.623	-1471.110
$Fe_2SiO_4(s2) = Fe_2SiO_4(l)$	($_mH^\circ(1090)=$	70.299±4.057	70.358	-1471.025)
Enthalpy of formation, $\Delta_f H^\circ(298)$, from weighted, least-squares optimization				-1470.966 ±3.381

Table 7.26. Summary of data for magnetite by reaction. The second column shows the weighted results from this study. The third column gives the average of the third-law $\Delta_r H°(298)$ data for each reaction. The last column gives the $\Delta_f H°(298)$ for magnetite calculated from the averages. The last calculation assumes that all other data are correct. Compare these values with the last entry which was derived from this study.

Reaction	$\Delta_r H°(298)$ (kJ/mol)		$\Delta_f H°(298)$ (kJ/mol)
	This Study	Average for Reaction	Calculated from Average
$3\ Fe + 2\ O_2 = Fe_3O_4$	-1116.640±0.235	-1118.370	-1118.370
$0.25\ Fe_3O_4 + CO = 0.75\ Fe + CO_2$	-3.821±0.059	-----	-----
$0.25\ Fe_3O_4 + H_2 = 0.75\ Fe + H_2O(g)$	37.333±0.059	37.614	-1117.764
$2\ Fe_3O_4 = 6\ FeO + O_2$	660.458±2.511	660.318	-1116.570
$Fe_3O_4 + CO = 3\ FeO + CO_2$	47.262±1.256	47.489	-1116.867
$Fe_3O_4 + H_2 = 3\ FeO + H_2O(g)$	88.416±1.256	88.822	-1117.046
$Fe_3O_4 + Fe = 4\ FeO$	68.110±1.661	67.943	-1116.473
$Fe_3O_4 + 2\ Cu = 3\ FeO + Cu_2O$	159.612±1.277	-----	-----
$Fe_3O_4 + Ni = 3\ FeO + NiO$	89.965±1.312	89.480	-1116.155
$3\ Fe_2O_3 + H_2 = 2\ Fe_3O_4 + H_2O(g)$	-0.320±0.705	-1.485	-1117.223
$2\ Fe_3O_4 + 0.5\ O_2 = 3\ Fe_2O_3$	-241.506±0.705	-241.694	-1116.654

Table 7.26. Summary of data for magnetite by reaction. Continued.

Reaction	$_rH°(298)$ (kJ/mol) This Study	$_rH°(298)$ (kJ/mol) Average for Reaction	$_fH°(298)$ (kJ/mol) Calculated from Average
$3\ Fe_2O_3 + 2\ Cu = 2\ Fe_3O_4 + Cu_2O$	70.875±0.728	70.601	-1116.777
$3\ Fe_2O_3 + Fe = 2\ Fe_3O_4 + FeO$	-20.626±0.972	-20.684	-1116.669
$3\ Fe_2O_3 + Ni = 2\ Fe_3O_4 + NiO$	1.229±0.790	1.058	-1116.725
$2\ Fe_3O_4 + 3\ SiO_2 = 3\ Fe_2SiO_4(sl) + O_2$	532.187±4.000	-----	-----
$Fe_3O_4 + 1.5\ SiO_2 + CO = 1.5\ Fe_2SiO_4(sl) + CO_2$	-16.887±2.000	-14.667	-1118.860
$Fe_3O_4 + 1.5\ SiO_2 + H_2 = 1.5\ Fe_2SiO_4(sl) + H_2O(g)$	24.266±2.000	23.456	-1115.830
$Fe_3O_4 + 1.5\ SiO_2 + 2\ Cu = 1.5\ Fe_2SiO_4(sl) + Cu_2O$	-95.462±2.016	-----	-----
$Fe_3O_4 + 1.5\ SiO_2 + Fe = 1.5\ Fe_2SiO_4(sl) + FeO$	3.906±2.044	-----	-----
$2\ Fe + SiO_2 + 2\ Fe_3O_4 = Fe_2SiO_4(sl) + 6\ FeO$	93.545±2.839	-----	-----
Enthalpy of formation, $\Delta_fH°(298)$, from weighted, least-squares optimization			-1116.640 ~~±0.235~~ ±2.245

Table 8.01. Thermodynamic properties of graphite, C(s). The string "----" indicates that the property was not evaluated. The source of data is Garvin and others (1987).

T	V°	S°	$-[G^\circ_T-H^\circ_{298}]/T$	$[H^\circ_T-H^\circ_{298}]/T$	C°_p	$H^\circ_T-H^\circ_{298}$	Δ_fH°	Δ_fG°	$\log {}_fK^\circ$
K	cm³/mol	------------J/(mol·K)	------------	------------	------------	--------J/mol	--------	--------	
200.	----	3.091	6.401	-3.310	5.021	-662.	0.	0.	0.000
250.	----	4.396	5.868	-1.472	6.770	-368.	0.	0.	0.000
273.15	----	5.032	5.770	-0.740	7.610	-202.	0.	0.	0.000
298.15	----	5.738	5.738	0.000	8.513	0.	0.	0.	0.000
300.	----	5.791	5.738	0.053	8.580	16.	0.	0.	0.000
350.	----	7.245	5.849	1.397	10.314	489.	0.	0.	0.000
400.	----	8.728	6.116	2.612	11.906	1045.	0.	0.	0.000
450.	----	10.215	6.489	3.727	13.340	1677.	0.	0.	0.000
500.	----	11.687	6.935	4.752	14.617	2376.	0.	0.	0.000
550.	----	13.135	7.433	5.702	15.751	3136.	0.	0.	0.000
600.	----	14.549	7.968	6.582	16.755	3949.	0.	0.	0.000
650.	----	15.926	8.527	7.398	17.645	4809.	0.	0.	0.000
700.	----	17.263	9.104	8.160	18.433	5712.	0.	0.	0.000
750.	----	18.559	9.691	8.868	19.133	6651.	0.	0.	0.000
800.	----	19.815	10.285	9.530	19.755	7624.	0.	0.	0.000
850.	----	21.029	10.881	10.148	20.309	8626.	0.	0.	0.000
900.	----	22.204	11.478	10.727	20.802	9654.	0.	0.	0.000
950.	----	23.341	12.072	11.268	21.242	10705.	0.	0.	0.000
1000.	----	24.441	12.663	11.777	21.635	11777.	0.	0.	0.000
1050.	----	25.505	13.250	12.255	21.986	12868.	0.	0.	0.000
1100.	----	26.535	13.830	12.705	22.301	13975.	0.	0.	0.000
1150.	----	27.533	14.405	13.128	22.583	15097.	0.	0.	0.000
1200.	----	28.499	14.972	13.528	22.836	16233.	0.	0.	0.000
1250.	----	29.436	15.532	13.905	23.063	17381.	0.	0.	0.000
1300.	----	30.345	16.084	14.261	23.268	18539.	0.	0.	0.000
1350.	----	31.226	16.629	14.598	23.452	19707.	0.	0.	0.000
1400.	----	32.082	17.165	14.917	23.619	20884.	0.	0.	0.000
1450.	----	32.914	17.694	15.220	23.770	22069.	0.	0.	0.000
1500.	----	33.722	18.215	15.507	23.907	23261.	0.	0.	0.000
1550.	----	34.508	18.728	15.780	24.032	24459.	0.	0.	0.000
1600.	----	35.273	19.233	16.040	24.146	25664.	0.	0.	0.000
1650.	----	36.018	19.730	16.287	24.251	26874.	0.	0.	0.000
1700.	----	36.743	20.220	16.523	24.348	28089.	0.	0.	0.000
1750.	----	37.450	20.702	16.747	24.438	29308.	0.	0.	0.000
1800.	----	38.140	21.177	16.962	24.522	30532.	0.	0.	0.000

Table 8.02. Thermodynamic properties of carbon monoxide, CO(g). The string "----" indicates that the property was not evaluated. The source of data is Garvin and others (1987).

T	V°	S°	$\frac{-[G^\circ_T-H^\circ_{298}]}{T}$	$\frac{[H^\circ_T-H^\circ_{298}]}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	----	186.034	200.326	-14.290	29.028	-2858.	-111291.	-128531.	33.568
250.	----	192.527	198.140	-5.612	29.139	-1403.	-110859.	-132893.	27.766
273.15	----	195.108	197.776	-2.669	29.143	-729.	-110690.	-134941.	25.804
298.15	----	197.660	197.660	0.000	29.146	0.	-110529.	-137168.	24.031
300.	----	197.841	197.661	0.180	29.146	54.	-110518.	-137333.	23.911
350.	----	202.336	198.016	4.320	29.196	1512.	-110270.	-141823.	21.166
400.	----	206.243	198.805	7.438	29.328	2975.	-110110.	-146343.	19.110
450.	----	209.709	199.828	9.880	29.539	4446.	-110029.	-150878.	17.513
500.	----	212.834	200.975	11.860	29.810	5930.	-110016.	-155418.	16.236
550.	----	215.690	202.185	13.505	30.123	7428.	-110062.	-159956.	15.191
600.	----	218.325	203.421	14.905	30.463	8943.	-110158.	-164488.	14.320
650.	----	220.778	204.663	16.115	30.817	10475.	-110295.	-169010.	13.582
700.	----	223.075	205.897	17.177	31.177	12024.	-110467.	-173520.	12.948
750.	----	225.238	207.115	18.123	31.534	13592.	-110668.	-178017.	12.398
800.	----	227.284	208.312	18.973	31.884	15178.	-110894.	-182500.	11.916
850.	----	229.227	209.486	19.741	32.224	16780.	-111140.	-186968.	11.489
900.	----	231.079	210.634	20.444	32.550	18400.	-111404.	-191421.	11.110
950.	----	232.847	211.757	21.089	32.862	20035.	-111682.	-195859.	10.769
1000.	----	234.540	212.854	21.686	33.158	21686.	-111972.	-200282.	10.461
1050.	----	236.165	213.926	22.239	33.438	23351.	-112272.	-204690.	10.183
1100.	----	237.726	214.973	22.754	33.700	25029.	-112581.	-209084.	9.928
1150.	----	239.230	215.995	23.235	33.946	26720.	-112897.	-213463.	9.696
1200.	----	240.680	216.993	23.687	34.175	28424.	-113220.	-217829.	9.482
1250.	----	242.079	217.969	24.110	34.388	30138.	-113548.	-222181.	9.284
1300.	----	243.432	218.922	24.509	34.584	31862.	-113880.	-226519.	9.101
1350.	----	244.740	219.854	24.886	34.765	33596.	-114217.	-230845.	8.932
1400.	----	246.008	220.766	25.241	34.930	35338.	-114558.	-235159.	8.774
1450.	----	247.236	221.658	25.579	35.080	37089.	-114902.	-239460.	8.626
1500.	----	248.428	222.530	25.897	35.216	38846.	-115250.	-243749.	8.488
1550.	----	249.584	223.384	26.200	35.338	40610.	-115600.	-248026.	8.358
1600.	----	250.708	224.221	26.487	35.446	42380.	-115954.	-252292.	8.236
1650.	----	251.800	225.040	26.760	35.542	44154.	-116311.	-256548.	8.121
1700.	----	252.863	225.843	27.020	35.625	45934.	-116671.	-260792.	8.013
1750.	----	253.896	226.630	27.267	35.696	47717.	-117035.	-265025.	7.910
1800.	----	254.903	227.401	27.502	35.755	49503.	-117402.	-269248.	7.813

Table 8.03. Thermodynamic properties of carbon dioxide, $CO_2(g)$. The string "----" indicates that the property was not evaluated. The source of data is Garvin and others (1987).

T	V°	S°	$\frac{-[G^\circ_T-H^\circ_{298}]}{T}$	$\frac{[H^\circ_T-H^\circ_{298}]}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
K	cm^3/mol	------------J/(mol·K)	------------	------------	------------	--------J/mol	--------	--------	
200.	----	199.965	217.032	-17.065	32.226	-3413.	-393392.	-394070.	102.918
250.	----	207.446	214.385	-6.940	34.866	-1735.	-393465.	-394230.	82.368
273.15	----	210.583	213.931	-3.346	35.990	-914.	-393489.	-394300.	75.401
298.15	----	213.786	213.786	0.000	37.148	0.	-393510.	-394373.	69.091
300.	----	214.016	213.786	0.230	37.231	69.	-393511.	-394378.	68.666
350.	----	219.918	214.248	5.671	39.375	1985.	-393543.	-394520.	58.878
400.	----	225.305	215.298	10.008	41.311	4003.	-393574.	-394658.	51.536
450.	----	230.273	216.689	13.584	43.059	6113.	-393612.	-394791.	45.825
500.	----	234.893	218.281	16.612	44.635	8306.	-393661.	-394920.	41.256
550.	----	239.215	219.990	19.225	46.060	10574.	-393722.	-395043.	37.517
600.	----	243.279	221.763	21.517	47.350	12910.	-393793.	-395160.	34.401
650.	----	247.116	223.567	23.549	48.520	15307.	-393873.	-395271.	31.764
700.	----	250.751	225.380	25.371	49.585	17760.	-393961.	-395375.	29.503
750.	----	254.206	227.188	27.019	50.555	20264.	-394056.	-395473.	27.543
800.	----	257.497	228.980	28.518	51.441	22814.	-394156.	-395564.	25.827
850.	----	260.641	230.751	29.891	52.252	25407.	-394260.	-395649.	24.313
900.	----	263.649	232.495	31.153	52.995	28038.	-394366.	-395727.	22.967
950.	----	266.533	234.211	32.321	53.677	30705.	-394475.	-395800.	21.762
1000.	----	269.302	235.897	33.405	54.304	33405.	-394584.	-395867.	20.678
1050.	----	271.966	237.552	34.414	54.881	36135.	-394694.	-395928.	19.696
1100.	----	274.531	239.175	35.356	55.412	38892.	-394804.	-395984.	18.803
1150.	----	277.005	240.766	36.239	55.902	41675.	-394914.	-396035.	17.988
1200.	----	279.394	242.326	37.068	56.353	44482.	-395023.	-396082.	17.241
1250.	----	281.703	243.855	37.848	56.770	47310.	-395132.	-396124.	16.553
1300.	----	283.937	245.354	38.583	57.153	50158.	-395239.	-396161.	15.918
1350.	----	286.101	246.823	39.278	57.507	53025.	-395346.	-396195.	15.329
1400.	----	288.198	248.264	39.934	57.834	55908.	-395451.	-396224.	14.783
1450.	----	290.233	249.676	40.557	58.134	58808.	-395556.	-396250.	14.274
1500.	----	292.209	251.061	41.147	58.411	61721.	-395660.	-396272.	13.799
1550.	----	294.128	252.420	41.708	58.665	64648.	-395764.	-396291.	13.355
1600.	----	295.994	253.752	42.242	58.899	67588.	-395867.	-396306.	12.938
1650.	----	297.810	255.060	42.750	59.113	70538.	-395970.	-396318.	12.546
1700.	----	299.578	256.343	43.235	59.309	73499.	-396073.	-396327.	12.177
1750.	----	301.300	257.603	43.697	59.488	76469.	-396177.	-396333.	11.830
1800.	----	302.978	258.841	44.137	59.651	79447.	-396281.	-396336.	11.501

Table 8.04. Thermodynamic properties of copper, Cu(s,l). The string "----" indicates that the property was not evaluated. The source of data is Cox and others (1987).

T	V°	S°	$\frac{-[G^\circ_T - H^\circ_{298}]}{T}$	$\frac{[H^\circ_T - H^\circ_{298}]}{T}$	C°_p	$H^\circ_T - H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log $_fK^\circ$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	----	23.732	35.325	-11.595	22.668	-2319.	0.	0.	0.000
250.	----	28.902	33.539	-4.636	23.676	-1159.	0.	0.	0.000
273.15	----	31.016	33.236	-2.219	24.068	-606.	0.	0.	0.000
298.15	----	33.140	33.140	0.000	24.436	0.	0.	0.	0.000
300.	----	33.292	33.141	0.150	24.461	45.	0.	0.	0.000
350.	----	37.108	33.441	3.666	25.032	1283.	0.	0.	0.000
400.	----	40.478	34.114	6.365	25.440	2546.	0.	0.	0.000
450.	----	43.493	34.992	8.502	25.740	3826.	0.	0.	0.000
500.	----	46.218	35.980	10.238	25.978	5119.	0.	0.	0.000
550.	----	48.703	37.026	11.678	26.184	6423.	0.	0.	0.000
600.	----	50.990	38.095	12.895	26.383	7737.	0.	0.	0.000
650.	----	53.110	39.170	13.940	26.589	9061.	0.	0.	0.000
700.	----	55.089	40.237	14.851	26.814	10396.	0.	0.	0.000
750.	----	56.947	41.290	15.657	27.065	11743.	0.	0.	0.000
800.	----	58.703	42.324	16.379	27.345	13103.	0.	0.	0.000
850.	----	60.369	43.336	17.033	27.657	14478.	0.	0.	0.000
900.	----	61.960	44.327	17.632	28.002	15869.	0.	0.	0.000
950.	----	63.484	45.296	18.188	28.381	17279.	0.	0.	0.000
1000.	----	64.950	46.242	18.708	28.794	18708.	0.	0.	0.000
1050.	----	66.366	47.167	19.199	29.240	20159.	0.	0.	0.000
1100.	----	67.737	48.071	19.666	29.718	21633.	0.	0.	0.000
1150.	----	69.069	48.955	20.114	30.228	23131.	0.	0.	0.000
1200.	----	70.367	49.820	20.547	30.767	24656.	0.	0.	0.000
1250.	----	71.634	50.667	20.966	31.336	26208.	0.	0.	0.000
1300.	----	72.875	51.498	21.377	31.933	27790.	0.	0.	0.000
1350.	----	74.091	52.312	21.779	32.556	29402.	0.	0.	0.000
1357.6	----	74.274	52.434	21.840	32.653	29650.	0.	0.	0.000
Crystal = Liquid									
1357.6	----	83.941	52.434	31.506	32.800	42773.	0.	0.	0.000
1400.	----	84.950	53.404	31.546	32.800	44164.	0.	0.	0.000
1450.	----	86.101	54.512	31.589	32.800	45804.	0.	0.	0.000
1500.	----	87.213	55.583	31.629	32.800	47444.	0.	0.	0.000
1550.	----	88.288	56.621	31.667	32.800	49084.	0.	0.	0.000
1600.	----	89.330	57.627	31.703	32.800	50724.	0.	0.	0.000
1650.	----	90.339	58.603	31.736	32.800	52364.	0.	0.	0.000
1700.	----	91.318	59.551	31.767	32.800	54004.	0.	0.	0.000
1750.	----	92.269	60.472	31.797	32.800	55644.	0.	0.	0.000
1800.	----	93.193	61.368	31.824	32.800	57284.	0.	0.	0.000

Table 8.05. Thermodynamic properties of tenorite, CuO(s). The string "----" indicates that the property was not evaluated. The source of data is this study.

T K	$V°$ cm^3/mol	$S°$	$-[G°_T-H°_{298}]/T$	$[H°_T-H°_{298}]/T$	$C°_p$	$H°_T-H°_{298}$	$_fH°$	$_fG°$	$\log {}_fK°$
		------------J/(mol·K)------------				--------J/mol--------			
200.	----	27.016	46.268	-19.250	34.857	-3850.	-155757.	-137065.	35.797
227.	----	31.720	44.258	-12.537	39.567	-2846.	-155765.	-134540.	30.958
2 s	----	0.088	0.091	0.079	0.523	18.	204.	199.	0.046
					T_N				
227.	----	31.720	44.258	-12.537	39.567	-2846.	-155765.	-134540.	30.958
250.	----	35.454	43.278	-7.824	39.086	-1956.	-155751.	-132390.	27.661
2 s	----	0.086	0.088	0.060	0.259	15.	205.	199.	0.042
273.15	----	38.979	42.766	-3.785	40.573	-1034.	-155721.	-130228.	24.903
298.15	----	42.602	42.602	0.000	42.145	0.	-155660.	-127897.	22.407
2 s	----	0.086	0.086	0.000	0.363	0.	209.	198.	0.035
300.	----	42.863	42.602	0.260	42.255	78.	-155654.	-127725.	22.238
350.	----	49.580	43.127	6.454	44.846	2259.	-155449.	-123085.	18.369
400.	----	55.702	44.322	11.380	46.792	4552.	-155165.	-118481.	15.472
450.	----	61.302	45.902	15.400	48.262	6930.	-154825.	-113915.	13.223
500.	----	66.448	47.703	18.746	49.400	9373.	-154446.	-109389.	11.428
2 s	----	0.203	0.102	0.130	0.347	65.	256.	182.	0.019
550.	----	71.200	49.626	21.575	50.308	11866.	-154041.	-104903.	9.963
600.	----	75.611	51.610	24.002	51.058	14401.	-153618.	-100455.	8.745
650.	----	79.724	53.616	26.108	51.699	16970.	-153181.	-96042.	7.718
700.	----	83.576	55.620	27.956	52.268	19569.	-152736.	-91663.	6.840
750.	----	87.200	57.605	29.595	52.788	22196.	-152286.	-87317.	6.081
2 s	----	0.263	0.133	0.175	0.522	131.	315.	141.	0.010
800.	----	90.623	59.563	31.060	53.277	24848.	-151833.	-83000.	5.419
850.	----	93.867	61.486	32.380	53.749	27523.	-151380.	-78712.	4.837
900.	----	96.952	63.372	33.580	54.211	30222.	-150927.	-74450.	4.321
950.	----	99.896	65.217	34.679	54.671	32945.	-150477.	-70214.	3.861
1000.	----	102.712	67.022	35.690	55.133	35690.	-150029.	-66001.	3.447
2 s	----	0.294	0.156	0.193	0.508	193.	346.	97.	0.005
1050.	----	105.413	68.786	36.627	55.601	38458.	-149586.	-61811.	3.075
1100.	----	108.010	70.510	37.500	56.078	41250.	-149148.	-57641.	2.737
1150.	----	110.514	72.196	38.318	56.565	44066.	-148716.	-53492.	2.430
1200.	----	112.932	73.843	39.089	57.063	46907.	-148290.	-49361.	2.149
1250.	----	115.271	75.453	39.818	57.573	49772.	-147871.	-45247.	1.891
2 s	----	0.279	0.170	0.191	1.527	239.	335.	90.	0.004
1300.	----	117.539	77.029	40.511	58.095	52664.	-147460.	-41150.	1.653
1350.	----	119.742	78.570	41.172	58.631	55582.	-147057.	-37069.	1.434
1357.6	----	120.071	78.802	41.270	58.713	56028.	-146996.	-36450.	1.402
				-Cu(Crystal = Liquid)-					
1357.6	----	120.071	78.802	41.270	58.713	56028.	-160119.	-36450.	1.402
1400.	----	121.884	80.079	41.805	59.179	58527.	-159780.	-32593.	1.216
1450.	----	123.971	81.557	42.414	59.741	61500.	-159356.	-28058.	1.011
1500.	----	126.006	83.004	43.001	60.315	64502.	-158908.	-23538.	0.820
2 s	----	0.529	0.175	0.475	3.271	713.	710.	138.	0.005

Table 8.06. Thermodynamic properties of cuprite and liquid dicuprous oxide, $Cu_2O(s,l)$. The string "----" indicates that the property was not evaluated. The source of data is this study.

T	V°	S°	$-[G^\circ_T-H^\circ_{298}]/T$	$[H^\circ_T-H^\circ_{298}]/T$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
K	cm³/mol	------------J/(mol·K)	------------	------------		--------J/mol	--------		
200.	----	69.146	97.841	-28.695	53.609	-5739.	-170298.	-155286.	40.556
250.	----	81.689	93.384	-11.696	58.765	-2924.	-170531.	-151503.	31.654
2 s	----	0.080	0.090	0.044	0.232	11.	221.	217.	0.045
273.15	----	86.979	92.619	-5.638	60.693	-1540.	-170592.	-149738.	28.634
298.15	----	92.374	92.374	0.000	62.501	0.	-170631.	-147828.	25.898
2 s	----	0.089	0.089	0.000	0.253	0.	226.	216.	0.038
300.	----	92.761	92.375	0.387	62.624	116.	-170633.	-147686.	25.714
350.	----	102.643	93.149	9.494	65.534	3323.	-170639.	-143860.	21.469
400.	----	111.548	94.902	16.645	67.798	6658.	-170575.	-140038.	18.287
450.	----	119.642	97.208	22.436	69.628	10096.	-170456.	-136228.	15.813
500.	----	127.060	99.827	27.232	71.165	13616.	-170293.	-132433.	13.835
2 s	----	0.202	0.101	0.138	0.394	69.	279.	198.	0.021
550.	----	133.907	102.618	31.289	72.502	17209.	-170093.	-128656.	12.219
600.	----	140.268	105.494	34.773	73.702	20864.	-169862.	-124899.	10.873
650.	----	146.211	108.400	37.811	74.808	24577.	-169606.	-121163.	9.737
700.	----	151.793	111.302	40.491	75.851	28344.	-169329.	-117446.	8.764
750.	----	157.061	114.179	42.883	76.850	32162.	-169035.	-113751.	7.922
2 s	----	0.296	0.140	0.184	0.363	138.	341.	153.	0.011
800.	----	162.052	117.016	45.036	77.823	36029.	-168727.	-110075.	7.187
850.	----	166.799	119.806	46.993	78.778	39944.	-168409.	-106419.	6.540
900.	----	171.328	122.543	48.784	79.725	43906.	-168084.	-102782.	5.965
950.	----	175.664	125.226	50.438	80.669	47916.	-167755.	-99163.	5.452
1000.	----	179.826	127.853	51.973	81.613	51973.	-167425.	-95561.	4.992
2 s	----	0.308	0.171	0.192	0.921	192.	367.	112.	0.006
1050.	----	183.831	130.423	53.408	82.561	56078.	-167097.	-91976.	4.575
1100.	----	187.693	132.939	54.754	83.516	60229.	-166773.	-88407.	4.198
1150.	----	191.427	135.402	56.025	84.478	64429.	-166455.	-84852.	3.854
1200.	----	195.043	137.812	57.231	85.449	68677.	-166147.	-81311.	3.539
1250.	----	198.551	140.171	58.379	86.429	72974.	-165849.	-77782.	3.250
2 s	----	0.426	0.185	0.353	1.698	441.	509.	107.	0.004
1300.	----	201.960	142.483	59.477	87.419	77320.	-165565.	-74265.	2.984
1350.	----	205.278	144.747	60.530	88.419	81716.	-165296.	-70758.	2.738
1357.6	----	205.775	145.088	60.687	88.572	82389.	-165256.	-70226.	2.702
				-Cu(Crystal = Liquid)-					
1357.6	----	205.775	145.088	60.687	88.572	82389.	-191503.	-70226.	2.702
1400.	----	208.512	146.967	61.545	89.430	86163.	-191280.	-66442.	2.479
1450.	----	211.668	149.144	62.523	90.451	90659.	-190972.	-61989.	2.233
1500.	----	214.751	151.280	63.472	91.482	95208.	-190617.	-57547.	2.004
2 s	----	0.728	0.208	0.625	2.539	937.	935.	198.	0.007
1516.7	----	215.766	151.984	63.782	91.828	96738.	-190488.	-56066.	1.931
				Crystal = Liquid					
1516.7	----	259.082	151.984	107.098	99.614	162435.	-124791.	-56066.	1.931
1550.	----	261.245	154.308	106.937	99.614	165752.	-124269.	-54563.	1.839
1600.	----	264.408	157.700	106.708	99.614	170733.	-123487.	-52327.	1.708
1650.	----	267.473	160.980	106.493	99.614	175713.	-122708.	-50115.	1.586
1700.	----	270.447	164.156	106.291	99.614	180694.	-121932.	-47927.	1.473
1750.	----	273.334	167.234	106.100	99.614	185675.	-121158.	-45762.	1.366
2 s	----	5.182	0.364	4.890	43.761	8557.	8560.	574.	0.017
1800.	----	276.140	170.221	105.919	99.614	190655.	-120387.	-43618.	1.266
2 s	----	6.400	0.493	5.958	43.761	10724.	10726.	842.	0.024

Table 8.07. Thermodynamic properties of iron (s1=alpha=bcc; s2=gamma=fcc), Fe(s1,s2). The string "----" indicates that the property was not evaluated. The sources of data are Chase and others (1985) for the thermodynamic data and this study for the volumes.

T	V°	S°	$\frac{-[G^\circ_T-H^\circ_{298}]}{T}$	$\frac{[H^\circ_T-H^\circ_{298}]}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log $_fK^\circ$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	7.068	17.977	29.510	-11.535	21.688	-2307.	0.	0.	0.000
250.	7.078	23.032	27.721	-4.688	23.589	-1172.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
273.15	7.083	25.154	27.414	-2.259	24.324	-617.	0.	0.	0.000
298.15	7.089	27.316	27.316	0.000	25.054	0.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
300.	7.090	27.471	27.316	0.153	25.106	46.	0.	0.	0.000
350.	7.102	31.441	27.627	3.814	26.398	1335.	0.	0.	0.000
400.	7.116	35.041	28.332	6.708	27.527	2683.	0.	0.	0.000
450.	7.131	38.343	29.263	9.080	28.561	4086.	0.	0.	0.000
500.	7.146	41.405	30.326	11.078	29.568	5539.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
550.	7.162	44.271	31.465	12.805	30.606	7043.	0.	0.	0.000
600.	7.179	46.981	32.646	14.335	31.728	8601.	0.	0.	0.000
650.	7.196	49.569	33.849	15.720	32.983	10218.	0.	0.	0.000
700.	7.214	52.065	35.061	17.003	34.421	11902.	0.	0.	0.000
750.	7.232	54.495	36.276	18.219	36.100	13664.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
800.	7.250	56.887	37.490	19.397	38.099	15518.	0.	0.	0.000
850.	7.268	59.267	38.701	20.567	40.545	17482.	0.	0.	0.000
900.	7.287	61.669	39.910	21.759	43.673	19583.	0.	0.	0.000
950.	7.306	64.140	41.120	23.020	48.029	21869.	0.	0.	0.000
1000.	7.325	66.770	42.336	24.435	55.482	24435.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
1042.	7.341	69.327	43.370	25.957	72.503	27047.	0.	0.	0.000
					T_C				
1042.	7.341	69.327	43.370	25.957	72.503	27047.	0.	0.	0.000
1050.	7.344	69.786	43.570	26.216	57.300	27527.	0.	0.	0.000
1100.	7.363	72.106	44.816	27.290	45.636	30019.	0.	0.	0.000
1150.	7.382	74.048	46.046	28.003	42.161	32203.	0.	0.	0.000
1184.	7.396	75.257	46.868	28.389	40.859	33613.	0.	0.	0.000
				Fe(alpha) = Fe(gamma)					
1184.	7.297	76.016	46.868	29.149	33.862	34512.	0.	0.	0.000
1200.	7.305	76.472	47.259	29.212	33.995	35055.	0.	0.	0.000
1250.	7.331	77.868	48.456	29.412	34.412	36765.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
1300.	7.357	79.226	49.613	29.612	34.828	38496.	0.	0.	0.000
1350.	7.382	80.548	50.735	29.813	35.244	40248.	0.	0.	0.000
1400.	7.408	81.837	51.823	30.015	35.660	42021.	0.	0.	0.000
1450.	7.434	83.096	52.879	30.217	36.077	43814.	0.	0.	0.000
1500.	7.461	84.326	53.907	30.419	36.493	45628.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
1550.	7.487	85.529	54.908	30.621	36.909	47463.	0.	0.	0.000
1600.	7.513	86.708	55.883	30.824	37.326	49319.	0.	0.	0.000
1650.	7.539	87.863	56.835	31.028	37.742	51196.	0.	0.	0.000
1665.	7.547	88.205	57.116	31.089	37.867	51763.	0.	0.	0.000
				Fe(gamma) = Fe(alpha)					
1665.	7.584	88.707	57.116	31.592	41.022	52600.	0.	0.	0.000
1700.	7.598	89.566	57.775	31.791	41.493	54044.	0.	0.	0.000
1750.	7.617	90.779	58.701	32.078	42.212	56136.	0.	0.	0.000
2 s	0.003	----	----	----	----	----	0.	0.	0.000
1800.	7.637	91.978	59.609	32.370	42.981	58266.	0.	0.	0.000
2 s	0.003	----	----	----	----	----	0.	0.	0.000

Table 8.08. Thermodynamic properties of ferrous oxide, FeO(s). The string "----" indicates that the property was not evaluated. The source of data is this study.

T	V°	S°	$\frac{-[G^\circ_T-H^\circ_{298}]}{T}$	$\frac{[H^\circ_T-H^\circ_{298}]}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	Δ_fH°	Δ_fG°	$\log {}_fK^\circ$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	12.225	45.385	67.664	-22.280	45.142	-4456.	-262847.	-248980.	65.026
250.	12.226	55.277	64.231	-8.952	45.301	-2238.	-262493.	-245556.	51.305
2 s	0.005	0.809	0.696	0.140	0.798	35.	949.	747.	0.156
273.15	12.229	59.342	63.646	-4.305	46.478	-1176.	-262324.	-243995.	46.658
298.15	12.232	63.459	63.459	0.000	47.529	0.	-262133.	-242326.	42.454
2 s	0.004	0.705	0.705	0.000	0.674	0.	923.	713.	0.124
300.	12.233	63.754	63.460	0.293	47.598	88.	-262118.	-242203.	42.170
350.	12.243	71.211	64.046	7.166	49.095	2508.	-261724.	-238915.	35.655
400.	12.256	77.837	65.363	12.472	50.097	4989.	-261338.	-235683.	30.776
450.	12.272	83.781	67.085	16.696	50.813	7513.	-260975.	-232498.	26.987
500.	12.290	89.164	69.028	20.136	51.360	10068.	-260644.	-229352.	23.960
2 s	0.007	0.425	0.641	0.256	0.649	128.	824.	612.	0.063
550.	12.311	94.080	71.085	22.995	51.806	12647.	-260353.	-226237.	21.486
600.	12.333	98.605	73.193	25.412	52.189	15247.	-260108.	-223147.	19.426
650.	12.356	102.796	75.311	27.486	52.535	17866.	-259915.	-220075.	17.685
700.	12.380	106.701	77.415	29.286	52.859	20500.	-259784.	-217016.	16.194
750.	12.406	110.359	79.491	30.868	53.171	23151.	-259725.	-213963.	14.901
2 s	0.007	0.214	0.522	0.367	0.621	275.	708	548.	0.038
800.	12.432	113.800	81.528	32.271	53.477	25817.	-259751.	-210912.	13.771
839.15	12.453	116.361	83.094	33.267	53.715	27916.	-259842.	-208520.	12.979
2 s	0.007	0.161	0.482	0.384	0.609	322.	673.	538.	0.033
------------------- Iron(alpha) - Wustite Solid Solution - Magnetite Coexistance -------------------									
839.15	12.453	116.361	83.094	33.267	53.715	27916.	-259842.	-208520.	12.979
850.	12.459	117.051	83.523	33.528	53.781	28499.	-259881.	-207856.	12.773
900.	12.487	120.134	85.472	34.662	54.086	31196.	-260141.	-204789.	11.885
950.	12.515	123.067	87.374	35.692	54.393	33907.	-260576.	-201703.	11.090
1000.	12.544	125.864	89.230	36.635	54.705	36635.	-261283.	-198588.	10.373
2 s	0.006	0.105	0.416	0.396	0.535	396.	638.	533.	0.027
1050.	12.573	128.541	91.038	37.503	55.021	39378.	-262507.	-195425.	9.722
1100.	12.602	131.108	92.802	38.306	55.343	42137.	-263120.	-192214.	9.127
1150.	12.631	133.575	94.521	39.054	55.669	44912.	-263414.	-188984.	8.584
1184.	12.651	135.201	95.666	39.535	55.894	46809.	-263532.	-186782.	8.240
- - - - - - - - - - - - - - - - - - -Fe(alpha) = Fe(gamma)- - - - - - - - - - - - - - - - - - - -									
1184.	12.651	135.201	95.666	39.535	55.894	46809.	-264431.	-186782.	8.240
1200.	12.661	135.952	96.198	39.753	56.001	47704.	-264364.	-185733.	8.085
1250.	12.691	138.245	97.834	40.410	56.338	50513.	-264161.	-182461.	7.624
2 s	0.004	0.095	0.332	0.370	0.415	462.	652.	534.	0.022
1300.	12.721	140.461	99.432	41.029	56.680	53338.	-263965.	-179196.	7.200
1350.	12.751	142.606	100.991	41.616	57.026	56181.	-263777.	-175940.	6.807
1400.	12.782	144.687	102.515	42.172	57.378	59041.	-263595.	-172690.	6.443
1450.	12.812	146.706	104.004	42.703	57.734	61919.	-263421.	-169446.	6.104
1500.	12.843	148.670	105.460	43.209	58.095	64814.	-263252.	-166209.	5.788
2 s	0.007	0.104	0.273	0.301	0.961	451.	695.	539.	0.018
1550.	12.873	150.581	106.885	43.695	58.460	67728.	-263089.	-162977.	5.492
1600.	12.904	152.442	108.280	44.162	58.829	70660.	-262932.	-159750.	5.215
1650.	12.935	154.258	109.646	44.613	59.202	73611.	-262780.	-156528.	4.955
1665.	12.944	154.795	110.050	44.745	59.315	74500.	-262735.	-155562.	4.880
- - - - - - - - - - - - - - - - - - -Fe(gamma) = Fe(alpha)- - - - - - - - - - - - - - - - - - - -									
1665.	12.944	154.795	110.050	44.745	59.315	74500.	-263571.	-155562.	4.880
1700.	12.966	156.031	110.984	45.048	59.579	76581.	-263582.	-153291.	4.710
1750.	12.996	157.764	112.296	45.468	59.959	79569.	-263613.	-150047.	4.479
2 s	0.011	0.270	0.239	0.291	1.988	509.	1024.	552.	0.016
1800.	13.027	159.458	113.582	45.876	60.343	82577.	-263665.	-146802.	4.260
2 s	0.012	0.324	0.235	0.314	2.229	565.	1144.	561.	0.016

Table 8.09. Thermodynamic properties of hematite, Fe_2O_3. The string "----" indicates that the property was not evaluated. The source of data is this study.

T	$V°$	$S°$	$-[G°_T-H°_{298}]/T$	$[H°_T-H°_{298}]/T$	$C°_p$	$H°_T-H°_{298}$	$\Delta_f H°$	$\Delta_f G°$	$\log {}_f K°$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	30.217	51.289	96.233	-44.945	76.227	-8989.	-825002.	-770022.	201.105
250.	30.244	70.131	89.138	-19.008	92.516	-4752.	-825220.	-756240.	158.004
2 s	0.019	0.049	0.060	0.020	0.111	5.	3154.	3142.	0.656
273.15	30.258	78.596	87.887	-9.292	98.604	-2538.	-825132.	-749856.	143.392
298.15	30.275	87.483	87.483	0.000	104.292	0.	-824929.	-742974.	130.163
2 s	0.014	0.059	0.059	0.000	0.121	0.	3158.	3141.	0.550
300.	30.277	88.129	87.485	0.643	104.680	193.	-824910.	-742466.	129.272
350.	30.314	104.980	88.795	16.186	113.758	5665.	-824227.	-728775.	108.761
400.	30.357	120.644	91.809	28.835	120.727	11534.	-823295.	-715200.	93.394
450.	30.402	135.196	95.831	39.364	126.293	17714.	-822194.	-701753.	81.466
500.	30.450	148.750	100.453	48.296	130.947	24148.	-820981.	-688434.	71.919
2 s	0.013	0.110	0.065	0.066	0.193	33.	3185.	3130.	0.327
550.	30.501	161.425	105.426	56.000	135.041	30800.	-819690.	-675242.	64.128
600.	30.555	173.340	110.594	62.745	138.835	37647.	-818349.	-662169.	57.646
650.	30.610	184.599	115.857	68.742	142.540	44682.	-816974.	-649210.	52.170
700.	30.666	195.300	121.153	74.147	146.358	51903.	-815580.	-636357.	47.485
750.	30.724	205.537	126.439	79.097	150.514	59323.	-814172.	-623604.	43.431
2 s	0.011	0.158	0.082	0.095	0.168	71.	3225.	3107.	0.216
800.	30.783	215.400	131.693	83.707	155.345	66966.	-812753.	-610946.	39.890
850.	30.842	224.993	136.900	88.093	161.491	74879.	-811309.	-598377.	36.771
900.	30.903	234.460	142.057	92.402	170.582	83162.	-809794.	-585895.	34.004
950.	30.964	244.087	147.172	96.915	187.995	92069.	-808045.	-573502.	31.533
955.53	30.971	245.187	147.736	97.451	191.034	93117.	-807819.	-572137.	31.276
2 s	0.008	0.175	0.096	0.105	0.741	100.	3255.	3088.	0.169
					T_N				
955.53	30.971	245.187	147.736	97.451	191.034	93117.	-807819.	-572137.	31.276
1000.	31.026	252.396	152.235	100.161	151.130	100161.	-807691.	-561177.	29.312
2 s	0.009	0.178	0.099	0.104	0.452	104.	3263.	3085.	0.161
1050.	31.088	259.632	157.179	102.453	146.379	107576.	-809084.	-548822.	27.302
1100.	31.151	266.399	161.991	104.407	144.801	114848.	-809436.	-536417.	25.472
1150.	31.214	272.823	166.671	106.152	144.383	122075.	-809233.	-524010.	23.801
1184.	31.257	277.030	169.780	107.250	144.414	126984.	-808957.	-515581.	22.745
				-Fe(alpha)	= Fe(gamma)-				
1184.	31.257	277.030	169.780	107.250	144.414	126984.	-810757.	-515581.	22.745
1200.	31.278	278.969	171.223	107.746	144.481	129295.	-810387.	-511595.	22.269
1250.	31.341	284.874	175.652	109.222	144.822	136527.	-809259.	-499169.	20.859
2 s	0.018	0.172	0.107	0.118	0.801	147.	3293.	3078.	0.128
1300.	31.405	290.562	179.963	110.599	145.286	143779.	-808165.	-486787.	19.559
1350.	31.469	296.055	184.161	111.894	145.813	151057.	-807099.	-474446.	18.357
1400.	31.533	301.368	188.253	113.115	146.377	158361.	-806058.	-462145.	17.242
1450.	31.597	306.515	192.243	114.272	146.964	165695.	-805040.	-449880.	16.206
1500.	31.662	311.507	196.135	115.372	147.567	173058.	-804044.	-437651.	15.240
2 s	0.033	0.270	0.110	0.238	1.151	357.	3500.	3094.	0.107
1550.	31.726	316.356	199.936	116.421	148.184	180452.	-803069.	-425454.	14.337
1600.	31.791	321.071	203.648	117.423	148.813	187877.	-802112.	-413288.	13.492
1650.	31.855	325.660	207.276	118.384	149.453	195333.	-801174.	-401152.	12.699
1665.	31.874	327.013	208.349	118.664	149.648	197576.	-800896.	-397516.	12.471
				-Fe(gamma)	= Fe(alpha)-				
1665.	31.874	327.013	208.349	118.664	149.648	197576.	-802570.	-397516.	12.471
1700.	31.920	330.131	210.824	119.307	150.105	202822.	-802154.	-389006.	11.952
1750.	31.984	334.492	214.295	120.197	150.769	210344.	-801598.	-376863.	11.249
2 s	0.048	0.444	0.120	0.387	1.505	677.	3932.	3155.	0.094
1800.	32.049	338.748	217.693	121.055	151.444	217899.	-801091.	-364735.	10.584
2 s	0.052	0.484	0.124	0.418	1.576	752.	4045.	3174.	0.092

Table 8.10. Thermodynamic properties of fayalite and liquid diferrous silicate, Fe_2SiO_4(sl,l). The string "----" indicates that the property was not evaluated. The source of data is this study.

T	V°	S°	$-[G^\circ_T-H^\circ_{298}]/T$	$[H^\circ_T-H^\circ_{298}]/T$	C°_p	$H^\circ_T-H^\circ_{298}$	Δ_fH°	Δ_fG°	$\log {}_fK^\circ$
K	cm³/mol	J/(mol·K)				J/mol			
200.	46.068	104.146	162.162	-58.015	101.983	-11603.	-1477211.	-1411125.	368.540
250.	46.117	128.819	153.054	-24.236	119.116	-6059.	-1477703.	-1394536.	291.366
2 s	0.024	1.012	1.011	0.040	0.214	10.	1324.	1116.	0.233
273.15	46.141	139.662	151.462	-11.799	125.714	-3223.	-1477766.	-1386832.	265.199
298.15	46.169	150.949	150.949	0.000	132.017	0.	-1477733.	-1378509.	241.504
2 s	0.024	1.011	1.011	0.000	0.219	0.	1324.	1078.	0.189
300.	46.171	151.767	150.951	0.817	132.452	245.	-1477727.	-1377894.	239.908
350.	46.230	172.997	152.604	20.391	142.840	7137.	-1477393.	-1361277.	203.155
400.	46.293	192.627	156.396	36.230	151.049	14492.	-1476806.	-1344727.	175.600
450.	46.359	210.813	161.445	49.369	157.642	22216.	-1476047.	-1328261.	154.177
500.	46.428	227.709	167.237	60.472	163.017	30236.	-1475177.	-1311886.	137.049
2 s	0.024	1.022	1.011	0.146	0.684	73.	1340.	927.	0.097
550.	46.499	243.461	173.458	70.004	167.456	38502.	-1474243.	-1295602.	123.043
600.	46.572	258.196	179.912	78.283	171.163	46970.	-1473287.	-1279404.	111.380
650.	46.647	272.023	186.472	85.551	174.290	55608.	-1472347.	-1263286.	101.517
700.	46.724	285.039	193.052	91.987	176.948	64391.	-1471458.	-1247238.	93.068
750.	46.801	297.327	199.598	97.729	179.222	73297.	-1470656.	-1231251.	85.750
2 s	0.024	1.112	1.015	0.384	1.093	288.	1416.	751.	0.052
800.	46.880	308.957	206.072	102.885	181.180	82308.	-1469984.	-1215313.	79.350
850.	46.960	319.994	212.452	107.541	182.874	91410.	-1469487.	-1199413.	73.705
900.	47.040	330.489	218.720	111.769	184.344	100592.	-1469230.	-1183535.	68.689
950.	47.120	340.491	224.868	115.623	185.623	109842.	-1469310.	-1167662.	64.201
1000.	47.202	350.041	230.890	119.151	186.740	119151.	-1469928.	-1151773.	60.161
2 s	0.024	1.232	1.031	0.532	1.786	532.	1527.	616.	0.032
1050.	47.284	359.176	236.783	122.393	187.715	128513.	-1471580.	-1135829.	56.503
1100.	47.366	367.929	242.546	125.383	188.568	137921.	-1472015.	-1119826.	53.175
1150.	47.448	376.328	248.182	128.146	189.314	147368.	-1471823.	-1103821.	50.136
1184.	47.505	381.851	251.941	129.910	189.767	153813.	-1471538.	-1092944.	48.217
				-Fe(alpha) = Fe(gamma)-					
1184.	47.505	381.851	251.941	129.910	189.767	153813.	-1473337.	-1092944.	48.217
1200.	47.531	384.399	253.690	130.709	189.966	156851.	-1472960.	-1087807.	47.350
1250.	47.614	392.166	259.075	133.090	190.534	166363.	-1471807.	-1071782.	44.786
2 s	0.024	1.423	1.055	0.794	3.878	992.	1743.	606.	0.025
1300.	47.697	399.649	264.339	135.310	191.028	175903.	-1470693.	-1055803.	42.422
1350.	47.781	406.866	269.485	137.381	191.456	185465.	-1469619.	-1039867.	40.234
1400.	47.864	413.836	274.516	139.319	191.825	195047.	-1468588.	-1023969.	38.204
1450.	47.948	420.573	279.437	141.136	192.140	204647.	-1467601.	-1008107.	36.315
1490.	48.015	425.805	283.297	142.508	192.358	212337.	-1466845.	-995442.	34.896
				Crystal = Liquid					
1490.	50.798	484.898	283.297	201.601	226.834	300386.	-1378796.	-995442.	34.896
1500.	50.798	486.415	284.646	201.769	226.834	302654.	-1378267.	-992871.	34.574
2 s	0.657	2.473	1.091	2.055	2.072	3082.	3373.	799.	0.028
1550.	50.798	493.853	291.275	202.578	226.834	313996.	-1375657.	-980067.	33.027
1600.	50.798	501.055	297.719	203.336	226.834	325337.	-1373107.	-967347.	31.580
1650.	50.798	508.035	303.987	204.048	226.834	336679.	-1370614.	-954706.	30.223
1665.	50.798	510.087	305.834	204.253	226.834	340082.	-1369877.	-950928.	29.832
				-Fe(gamma) = Fe(alpha)-					
1665.	50.798	510.087	305.834	204.253	226.834	340082.	-1371550.	-950928.	29.832
1685.	50.798	512.796	308.275	204.521	226.834	344618.	-1370704.	-945881.	29.321
				-Si(Crystal = Liquid)-					
1685.	50.798	512.796	308.275	204.521	226.834	344618.	-1421255.	-945881.	29.321
1700.	50.798	514.806	310.088	204.718	226.834	348021.	-1420587.	-941652.	28.933
1750.	50.798	521.382	316.032	205.350	226.834	359363.	-1418415.	-927598.	27.687
2 s	0.657	2.498	1.174	1.791	2.072	3134.	3420.	1236.	0.037
1800.	50.798	527.772	321.825	205.947	226.834	370704.	-1416326.	-913604.	26.512
2 s	0.657	2.507	1.194	1.753	2.072	3155.	3439.	1341.	0.039

Table 8.11. Thermodynamic properties of diferrous silicate (spinel structure), Fe_2SiO_4(s2). The string "----" indicates that the property was not evaluated. The source of data is this study.

T	V°	S°	$-[G^\circ_T-H^\circ_{298}]/T$	$[H^\circ_T-H^\circ_{298}]/T$	C°_p	$H^\circ_T-H^\circ_{298}$	Δ_fH°	Δ_fG°	log $_fK^\circ$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	41.901	92.276	150.935	-58.660	103.685	-11732.	-1470572.	-1402112.	366.186
250.	41.996	117.361	141.742	-24.380	120.613	-6095.	-1470972.	-1384941.	289.362
2 s	0.060	3.693	3.637	0.680	4.904	170.	3381.	2563.	0.535
273.15	42.036	128.307	140.143	-11.836	126.519	-3233.	-1471009.	-1376972.	263.314
298.15	42.076	139.629	139.629	0.000	131.979	0.	-1470966.	-1368367.	239.727
2 s	0.049	3.637	3.637	0.000	2.544	0.	3381.	2413.	0.423
300.	42.079	140.446	139.631	0.817	132.351	245.	-1470960.	-1367730.	238.138
350.	42.151	161.536	141.277	20.260	141.113	7091.	-1470672.	-1350545.	201.554
400.	42.215	180.845	145.033	35.813	147.985	14325.	-1470206.	-1333414.	174.122
450.	42.270	198.608	150.012	48.596	153.568	21868.	-1469627.	-1316349.	152.795
500.	42.320	215.036	155.704	59.332	158.226	29666.	-1468980.	-1299353.	135.740
2 s	0.054	3.461	3.598	0.660	1.977	330.	3344.	1828.	0.191
550.	42.364	230.307	161.800	68.507	162.193	37679.	-1468298.	-1282423.	121.792
600.	42.403	244.570	168.110	76.460	165.628	45876.	-1467613.	-1265555.	110.174
650.	42.439	257.949	174.511	83.438	168.643	54235.	-1466953.	-1248744.	100.348
700.	42.471	270.547	180.925	89.621	171.318	62735.	-1466346.	-1231982.	91.930
750.	42.501	282.450	187.300	95.149	173.715	71362.	-1465824.	-1215261.	84.636
2 s	0.069	3.038	3.454	1.061	3.245	796.	3128.	1295.	0.090
800.	42.528	293.731	193.603	100.129	175.880	80103.	-1465422.	-1198570.	78.257
850.	42.554	304.454	199.811	104.644	177.850	88947.	-1465183.	-1181900.	72.629
900.	42.577	314.671	205.910	108.761	179.653	97885.	-1465169.	-1165238.	67.627
950.	42.600	324.430	211.893	112.537	181.312	106910.	-1465475.	-1148569.	63.151
1000.	42.621	333.769	217.755	116.014	182.847	116014.	-1466298.	-1131871.	59.122
2 s	0.153	2.717	3.241	1.709	6.060	1709.	2889.	1121.	0.059
1050.	42.641	342.725	223.494	119.230	184.272	125192.	-1468134.	-1115109.	55.472
1100.	42.660	351.329	229.111	122.218	185.601	134440.	-1468729.	-1098280.	52.152
1150.	42.678	359.607	234.606	125.001	186.845	143751.	-1468673.	-1081441.	49.120
1184.	42.690	365.062	238.274	126.789	187.647	150118.	-1468465.	-1069995.	47.204
				-Fe(alpha) = Fe(gamma)-					
1184.	42.690	365.062	238.274	126.789	187.647	150118.	-1470265.	-1069995.	47.204
1200.	42.696	367.584	239.981	127.602	188.013	153123.	-1469921.	-1064588.	46.339
1250.	42.713	375.281	245.240	130.041	189.113	162551.	-1468852.	-1047722.	43.781
2 s	0.270	3.166	3.007	2.764	9.438	3455.	3433.	1350.	0.056
1300.	42.730	382.719	250.386	132.333	190.151	172033.	-1467795.	-1030897.	41.421
1350.	42.746	389.914	255.421	134.493	191.134	181566.	-1466752.	-1014113.	39.238
1400.	42.763	396.882	260.349	136.533	192.067	191146.	-1465723.	-997368.	37.211
1450.	42.778	403.637	265.174	138.463	192.953	200771.	-1464709.	-980659.	35.326
1500.	42.794	410.193	269.900	140.293	193.798	210440.	-1463713.	-963984.	33.568
2 s	0.399	4.553	2.829	4.085	13.015	6128.	5475.	1984.	0.069
1550.	42.809	416.561	274.528	142.033	194.604	220151.	-1462735.	-947343.	31.925
1600.	42.825	422.752	279.064	143.688	195.375	229900.	-1461776.	-930733.	30.385
1650.	42.840	428.775	283.510	145.265	196.114	239688.	-1460838.	-914152.	28.939
1665.	42.845	430.551	284.827	145.724	196.329	242631.	-1460560.	-909184.	28.522
				-Fe(gamma) = Fe(alpha)-					
1665.	42.845	430.551	284.827	145.724	196.329	242631.	-1462234.	-909184.	28.522
1685.	42.851	432.897	286.570	146.326	196.612	246560.	-1461995.	-902542.	27.978
				-Si(Crystal = Liquid)-					
1685.	42.851	432.897	286.570	146.326	196.612	246560.	-1512546.	-902542.	27.978
1700.	42.855	434.640	287.869	146.771	196.822	249511.	-1512330.	-897112.	27.564
1750.	42.870	440.356	292.145	148.211	197.502	259369.	-1511641.	-879028.	26.237
2 s	0.534	6.518	2.809	5.567	16.684	9742.	8834.	3117.	0.093
1800.	42.885	445.929	296.339	149.589	198.156	269261.	-1511003.	-860962.	24.984
2 s	0.561	6.955	2.833	5.877	17.424	10578.	9641.	3412.	0.099

Table 8.12. Thermodynamic properties of magnetite, $Fe_3O_4(s)$. The string "----" indicates that the property was not evaluated. The source of data is this study.

T	V°	S°	$-[G^\circ_T-H^\circ_{298}]/T$	$[H^\circ_T-H^\circ_{298}]/T$	C°_p	$H^\circ_T-H^\circ_{298}$	Δ_fH°	Δ_fG°	$\log {}_fK^\circ$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	44.454	92.002	158.229	-66.225	116.906	-13245.	-1117228.	-1047448.	273.559
250.	44.491	120.204	147.838	-27.632	135.845	-6908.	-1117210.	-1029992.	215.200
2 s	0.011	0.322	0.320	0.064	0.460	16.	2243.	2163.	0.565
273.15	44.514	132.566	146.023	-13.458	143.317	-3676.	-1116997.	-1021924.	195.419
298.15	44.542	145.438	145.438	0.000	150.615	0.	-1116640.	-1013237.	177.511
2 s	0.012	0.320	0.320	0.000	0.280	0.	2245.	2150.	0.377
300.	44.544	146.371	145.440	0.930	151.126	279.	-1116609.	-1012596.	176.305
350.	44.610	170.633	147.328	23.306	163.563	8157.	-1115546.	-995339.	148.543
400.	44.687	193.166	151.667	41.500	173.861	16600.	-1114135.	-978259.	127.745
450.	44.773	214.166	157.457	56.709	182.717	25519.	-1112456.	-961373.	111.591
500.	44.867	233.838	164.122	69.716	190.768	34858.	-1110562.	-944685.	98.689
2 s	0.015	0.301	0.314	0.126	0.510	63.	2246.	2096.	0.219
550.	44.968	252.387	171.311	81.076	198.595	44592.	-1108477.	-928197.	88.151
600.	45.074	270.013	178.807	91.205	206.769	54723.	-1106207.	-911907.	79.387
650.	45.185	286.916	186.477	100.438	215.939	65285.	-1103731.	-895814.	71.987
700.	45.301	303.309	194.239	109.070	227.040	76349.	-1100998.	-879921.	65.659
750.	45.419	319.450	202.049	117.401	241.911	88051.	-1097900.	-864235.	60.189
2 s	0.013	0.290	0.289	0.219	0.645	164.	2241.	2024.	0.141
800.	45.541	335.750	209.894	125.856	265.932	100685.	-1094181.	-848774.	55.418
849.1	45.663	352.970	217.658	135.312	324.100	114893.	-1089082.	-833854.	51.296
2 s	0.012	0.288	0.277	0.245	2.601	208.	2244.	2000.	0.123
					T_N				
849.1	45.663	352.970	217.658	135.312	324.100	114893.	-1089082.	-833854.	51.296
850.	45.665	353.277	217.802	135.475	287.241	115154.	-1088992.	-833583.	51.225
900.	45.791	367.046	225.729	141.318	221.378	127186.	-1086686.	-818642.	47.512
950.	45.919	378.655	233.477	145.178	209.991	137919.	-1086257.	-803768.	44.193
1000.	46.048	389.306	241.006	148.300	205.912	148300.	-1087048.	-788885.	41.206
2 s	0.016	0.246	0.261	0.218	0.733	218.	2286.	2040.	0.106
1050.	46.179	399.311	248.308	151.003	204.474	158553.	-1089572.	-773922.	38.500
1100.	46.311	408.812	255.389	153.423	204.142	168765.	-1090355.	-758866.	36.035
1150.	46.443	417.889	262.259	155.630	204.304	178975.	-1090237.	-743799.	33.784
1184.	46.534	423.845	266.814	157.032	204.556	185926.	-1089935.	-733561.	32.362
				-Fe(alpha) = Fe(gamma)-					
1184.	46.534	423.845	266.814	157.032	204.556	185926.	-1092634.	-733561.	32.362
1200.	46.576	426.592	268.926	157.667	204.700	189200.	-1092130.	-728712.	31.719
1250.	46.710	434.959	275.401	159.558	205.217	199447.	-1090591.	-713601.	29.819
2 s	0.028	0.221	0.233	0.250	1.131	312.	2366.	2090.	0.087
1300.	46.845	443.019	281.694	161.325	205.806	209723.	-1089103.	-698551.	28.068
1350.	46.980	450.798	287.814	162.984	206.444	220029.	-1087663.	-683557.	26.448
1400.	47.115	458.318	293.769	164.549	207.124	230368.	-1086266.	-668616.	24.946
1450.	47.251	465.598	299.570	166.029	207.842	240742.	-1084911.	-653724.	23.549
1500.	47.387	472.657	305.222	167.435	208.596	251152.	-1083595.	-638878.	22.247
2 s	0.043	0.357	0.206	0.375	1.499	562.	2668.	2133.	0.074
1550.	47.523	479.510	310.734	168.775	209.389	261602.	-1082315.	-624075.	21.031
1600.	47.660	486.171	316.113	170.058	210.219	272092.	-1081068.	-609313.	19.892
1650.	47.796	492.653	321.365	171.287	211.087	282624.	-1079853.	-594590.	18.823
1665.	47.838	494.564	322.917	171.647	211.356	285793.	-1079494.	-590180.	18.515
				-Fe(gamma) = Fe(alpha)-					
1665.	47.838	494.564	322.917	171.647	211.356	285793.	-1082004.	-590180.	18.515
1700.	47.933	498.968	326.496	172.471	211.995	293201.	-1081516.	-579847.	17.816
1750.	48.070	505.126	331.512	173.614	212.942	303825.	-1080878.	-565101.	16.867
2 s	0.060	0.567	0.195	0.527	1.816	922.	3203.	2211.	0.066
1800.	48.207	511.139	336.419	174.720	213.928	314496.	-1080314.	-550373.	15.971
2 s	0.063	0.612	0.196	0.558	1.878	1004.	3335.	2233.	0.065

Table 8.13. Thermodynamic properties of hydrogen, $H_2(g)$. The string "----" indicates that the property was not evaluated. The source of data is Garvin and others (1987).

T	V°	S°	$-[G^\circ_T-H^\circ_{298}]/T$	$[H^\circ_T-H^\circ_{298}]/T$	C°_p	$H^\circ_T-H^\circ_{298}$	Δ_fH°	Δ_fG°	$\log {}_fK^\circ$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	----	119.412	133.284	-13.870	27.556	-2774.	0.	0.	0.000
250.	----	125.644	131.153	-5.508	28.324	-1377.	0.	0.	0.000
273.15	----	128.165	130.794	-2.629	28.607	-718.	0.	0.	0.000
298.15	----	130.680	130.680	0.000	28.832	0.	0.	0.	0.000
300.	----	130.859	130.681	0.177	28.846	53.	0.	0.	0.000
350.	----	135.327	131.033	4.294	29.096	1503.	0.	0.	0.000
400.	----	139.220	131.818	7.400	29.195	2960.	0.	0.	0.000
450.	----	142.661	132.836	9.824	29.229	4421.	0.	0.	0.000
500.	----	145.741	133.975	11.766	29.243	5883.	0.	0.	0.000
550.	----	148.529	135.173	13.356	29.262	7346.	0.	0.	0.000
600.	----	151.076	136.394	14.683	29.296	8810.	0.	0.	0.000
650.	----	153.423	137.615	15.809	29.350	10276.	0.	0.	0.000
700.	----	155.601	138.823	16.779	29.425	11745.	0.	0.	0.000
750.	----	157.634	140.010	17.624	29.520	13218.	0.	0.	0.000
800.	----	159.543	141.172	18.371	29.633	14697.	0.	0.	0.000
850.	----	161.343	142.306	19.038	29.763	16182.	0.	0.	0.000
900.	----	163.049	143.411	19.638	29.907	17674.	0.	0.	0.000
950.	----	164.670	144.488	20.182	30.065	19173.	0.	0.	0.000
1000.	----	166.216	145.536	20.680	30.233	20680.	0.	0.	0.000
1050.	----	167.695	146.556	21.139	30.411	22196.	0.	0.	0.000
1100.	----	169.114	147.549	21.565	30.598	23722.	0.	0.	0.000
1150.	----	170.479	148.517	21.962	30.792	25256.	0.	0.	0.000
1200.	----	171.794	149.459	22.334	30.992	26801.	0.	0.	0.000
1250.	----	173.063	150.378	22.685	31.197	28356.	0.	0.	0.000
1300.	----	174.290	151.275	23.016	31.407	29921.	0.	0.	0.000
1350.	----	175.480	152.149	23.330	31.624	31496.	0.	0.	0.000
1400.	----	176.634	153.003	23.631	31.838	33083.	0.	0.	0.000
1450.	----	177.755	153.837	23.917	32.058	34680.	0.	0.	0.000
1500.	----	178.845	154.653	24.193	32.281	36289.	0.	0.	0.000
1550.	----	179.907	155.450	24.457	32.505	37908.	0.	0.	0.000
1600.	----	180.943	156.231	24.712	32.731	39539.	0.	0.	0.000
1650.	----	181.954	156.995	24.958	32.959	41181.	0.	0.	0.000
1700.	----	182.941	157.744	25.197	33.188	42835.	0.	0.	0.000
1750.	----	183.906	158.478	25.429	33.417	44500.	0.	0.	0.000
1800.	----	184.851	159.197	25.654	33.648	46177.	0.	0.	0.000

Table 8.14. Thermodynamic properties of ice, water, and ideal gas, $H_2O(s,l,g)$. The string "----" indicates that the property was not evaluated. The source of data is Garvin and others (1987).

T	V°	S°	$-\frac{[G^\circ_T-H^\circ_{298}]}{T}$	$\frac{[H^\circ_T-H^\circ_{298}]}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
K	cm³/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	----	31.140	82.679	-51.540	28.139	-10308.	-291881.	-254877.	66.566
250.	----	38.123	73.071	-34.948	34.713	-8737.	-292436.	-245557.	51.305
273.15	----	41.330	70.245	-28.915	37.756	-7890.	-292595.	-241208.	46.125
				ice = water					
273.15	----	63.329	70.245	-6.916	75.887	-1889.	-286586.	-241208.	46.125
298.15	----	69.947	69.947	0.000	75.345	0.	-285782.	-237091.	41.536
300.	----	70.413	69.948	0.463	75.327	139.	-285723.	-236789.	41.228
350.	----	82.026	70.865	11.163	75.550	3907.	-284142.	-228758.	34.140
372.78	----	86.802	71.694*	15.108	75.932	5632.	-283419.	-225176.*	31.551*
				water = gas*					
372.78	----	196.381	71.706*	124.674	34.000	46476.	-242575.	-225181.*	31.552*
400.	----	198.784	80.273	118.510	34.202	47404.	-242849.	-223901.	29.238
450.	----	202.837	93.670	109.167	34.650	49125.	-243347.	-221502.	25.711
500.	----	206.515	104.773	101.742	35.175	50871.	-243834.	-219049.	22.883
550.	----	209.894	114.178	95.716	35.754	52644.	-244308.	-216547.	20.566
600.	----	213.031	122.286	90.745	36.368	54447.	-244766.	-214003.	18.630
650.	----	215.967	129.381	86.586	37.004	56281.	-245207.	-211422.	16.990
700.	----	218.733	135.665	83.067	37.652	58147.	-245629.	-208807.	15.581
750.	----	221.353	141.291	80.061	38.306	60046.	-246033.	-206163.	14.358
800.	----	223.846	146.374	77.473	38.959	61978.	-246419.	-203492.	13.286
850.	----	226.227	151.001	75.226	39.608	63942.	-246787.	-200798.	12.339
900.	----	228.509	155.244	73.266	40.252	65939.	-247137.	-198082.	11.496
950.	----	230.703	159.159	71.544	40.887	67967.	-247470.	-195348.	10.741
1000.	----	232.816	162.789	70.027	41.514	70027.	-247786.	-192596.	10.060
1050.	----	234.857	166.172	68.684	42.130	72118.	-248085.	-189829.	9.443
1100.	----	236.830	169.340	67.491	42.737	74240.	-248369.	-187049.	8.882
1150.	----	238.743	172.316	66.428	43.333	76392.	-248637.	-184255.	8.369
1200.	----	240.600	175.122	65.477	43.918	78573.	-248890.	-181451.	7.898
1250.	----	242.405	177.778	64.626	44.493	80783.	-249129.	-178636.	7.465
1300.	----	244.161	180.297	63.863	45.058	83022.	-249354.	-175811.	7.064
1350.	----	245.872	182.694	63.177	45.613	85289.	-249566.	-172979.	6.693
1400.	----	247.540	184.981	62.559	46.158	87583.	-249764.	-170139.	6.348
1450.	----	249.169	187.166	62.003	46.693	89905.	-249950.	-167292.	6.026
1500.	----	250.761	189.260	61.502	47.219	92253.	-250123.	-164438.	5.726
1550.	----	252.318	191.269	61.049	47.736	94626.	-250285.	-161579.	5.445
1600.	----	253.842	193.200	60.641	48.245	97026.	-250435.	-158715.	5.181
1650.	----	255.334	195.061	60.273	48.745	99451.	-250575.	-155847.	4.934
1700.	----	256.796	196.855	59.941	49.237	101900.	-250703.	-152975.	4.700
1750.	----	258.231	198.588	59.642	49.721	104374.	-250821.	-150098.	4.480
1800.	----	259.638	200.264	59.373	50.198	106872.	-250929.	-147219.	4.272

* NOTE: The Gibbs energy of formation and related functions are not identical at the 1-bar boiling temperature because the vapor phase is not an ideal gas. The temperature at which $H_2O(l)$ and $H_2O(g)$ have identical Gibbs energies at 1 bar is approximately 373.19 K.

Table 8.15. Thermodynamic properties of "steam" ideal gas, $H_2O(g)$. The string "----" indicates that the property was not evaluated. The source of data is Garvin and others (1987).

T	$V°$	$S°$	$\frac{-[G°_T-H°_{298}]}{T}$	$\frac{[H°_T-H°_{298}]}{T}$	$C°_p$	$H°_T-H°_{298}$	$\Delta_fH°$	$\Delta_fG°$	$\log {}_fK°$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	----	175.524	191.895	-16.370	32.830	-3274.	-240892.	-232766.	60.791
250.	----	182.931	189.387	-6.456	33.422	-1614.	-241358.	-230681.	48.197
273.15	----	185.895	188.967	-3.072	33.522	-839.	-241581.	-229682.	43.921
298.15	----	188.835	188.835	0.000	33.613	0.	-241827.	-228582.	40.046
300.	----	189.043	188.835	0.207	33.620	62.	-241845.	-228500.	39.785
350.	----	194.242	189.245	4.997	33.856	1749.	-242345.	-226237.	33.763
400.	----	198.784	190.160	8.625	34.202	3450.	-242849.	-223901.	29.238
450.	----	202.837	191.347	11.491	34.650	5171.	-243347.	-221502.	25.711
500.	----	206.515	192.683	13.832	35.175	6916.	-243834.	-219049.	22.883
550.	----	209.894	194.096	15.798	35.754	8689.	-244308.	-216547.	20.566
600.	----	213.031	195.544	17.487	36.368	10492.	-244766.	-214003.	18.630
650.	----	215.967	197.004	18.963	37.004	12326.	-245207.	-211422.	16.990
700.	----	218.733	198.458	20.274	37.652	14192.	-245629.	-208807.	15.581
750.	----	221.353	199.898	21.455	38.306	16091.	-246033.	-206163.	14.358
800.	----	223.846	201.317	22.529	38.959	18023.	-246419.	-203492.	13.286
850.	----	226.227	202.713	23.514	39.608	19987.	-246787.	-200798.	12.339
900.	----	228.509	204.083	24.427	40.252	21984.	-247137.	-198082.	11.496
950.	----	230.703	205.427	25.276	40.887	24012.	-247470.	-195348.	10.741
1000.	----	232.816	206.744	26.072	41.514	26072.	-247786.	-192596.	10.060
1050.	----	234.857	208.034	26.822	42.130	28163.	-248085.	-189829.	9.443
1100.	----	236.830	209.298	27.532	42.737	30285.	-248369.	-187049.	8.882
1150.	----	238.743	210.537	28.206	43.333	32437.	-248637.	-184255.	8.369
1200.	----	240.600	211.751	28.848	43.918	34618.	-248890.	-181451.	7.898
1250.	----	242.405	212.942	29.463	44.493	36829.	-249129.	-178636.	7.465
1300.	----	244.161	214.109	30.052	45.058	39067.	-249354.	-175811.	7.064
1350.	----	245.872	215.254	30.618	45.613	41334.	-249566.	-172979.	6.693
1400.	----	247.540	216.377	31.164	46.158	43629.	-249764.	-170139.	6.348
1450.	----	249.169	217.480	31.690	46.693	45950.	-249950.	-167292.	6.026
1500.	----	250.761	218.563	32.199	47.219	48298.	-250123.	-164438.	5.726
1550.	----	252.318	219.627	32.692	47.736	50672.	-250285.	-161579.	5.445
1600.	----	253.842	220.672	33.169	48.245	53071.	-250435.	-158715.	5.181
1650.	----	255.334	221.700	33.634	48.745	55496.	-250575.	-155847.	4.934
1700.	----	256.796	222.711	34.086	49.237	57946.	-250703.	-152975.	4.700
1750.	----	258.231	223.705	34.526	49.721	60420.	-250821.	-150098.	4.480
1800.	----	259.638	224.684	34.954	50.198	62918.	-250929.	-147219.	4.272

Table 8.16. Thermodynamic properties of nickel, Ni(s,l). The string "----" indicates that the property was not evaluated. The sources of data are Chase and others (1985) for the thermodynamic data and this study for the volumes.

T	$V°$	$S°$	$\frac{-[G°_T-H°_{298}]}{T}$	$\frac{[H°_T-H°_{298}]}{T}$	$C°_p$	$H°_T-H°_{298}$	$\Delta_f H°$	$\Delta_f G°$	$\log {}_f K°$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	6.533	20.238	32.225	-11.985	22.428	-2397.	0.	0.	0.000
250.	6.544	25.484	30.364	-4.880	24.552	-1220.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
273.15	6.550	27.693	30.045	-2.350	25.322	-642.	0.	0.	0.000
298.15	6.556	29.943	29.943	0.000	26.044	0.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
300.	6.556	30.104	29.943	0.160	26.093	48.	0.	0.	0.000
350.	6.569	34.220	30.266	3.954	27.300	1384.	0.	0.	0.000
400.	6.583	37.935	30.996	6.940	28.358	2776.	0.	0.	0.000
450.	6.598	41.335	31.958	9.378	29.400	4220.	0.	0.	0.000
500.	6.613	44.491	33.055	11.436	30.553	5718.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
550.	6.628	47.468	34.231	13.236	32.017	7280.	0.	0.	0.000
600.	6.644	50.346	35.455	14.892	34.495	8935.	0.	0.	0.000
631.	6.654	52.173	36.231	15.943	35.194	10060.	0.	0.	0.000
					T_N				
631.	6.654	52.173	36.231	15.943	35.194	10060.	0.	0.	0.000
650.	6.660	53.170	36.711	16.458	32.668	10698.	0.	0.	0.000
700.	6.676	55.533	37.973	17.560	31.436	12292.	0.	0.	0.000
750.	6.693	57.691	39.216	18.475	31.179	13856.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
800.	6.710	59.702	40.435	19.268	31.189	15414.	0.	0.	0.000
850.	6.727	61.597	41.624	19.973	31.331	16977.	0.	0.	0.000
900.	6.744	63.394	42.784	20.610	31.554	18549.	0.	0.	0.000
950.	6.761	65.107	43.914	21.193	31.831	20133.	0.	0.	0.000
1000.	6.779	66.748	45.015	21.732	32.147	21732.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
1050.	6.796	68.324	46.088	22.236	32.495	23348.	0.	0.	0.000
1100.	6.814	69.844	47.133	22.711	32.867	24982.	0.	0.	0.000
1150.	6.831	71.314	48.153	23.161	33.259	26635.	0.	0.	0.000
1200.	6.849	72.738	49.148	23.590	33.669	28308.	0.	0.	0.000
1250.	6.867	74.121	50.119	24.002	34.094	30002.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
1300.	6.884	75.467	51.068	24.398	34.532	31718.	0.	0.	0.000
1350.	6.902	76.779	51.996	24.782	34.982	33456.	0.	0.	0.000
1400.	6.920	78.059	52.904	25.155	35.444	35217.	0.	0.	0.000
1450.	6.938	79.311	53.793	25.517	35.915	37000.	0.	0.	0.000
1500.	6.956	80.537	54.665	25.872	36.395	38808.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
1550.	6.974	81.738	55.519	26.219	36.884	40640.	0.	0.	0.000
1600.	6.991	82.917	56.356	26.561	37.381	42497.	0.	0.	0.000
1650.	7.009	84.075	57.179	26.896	37.885	44378.	0.	0.	0.000
1700.	7.027	85.213	57.987	27.226	38.396	46285.	0.	0.	0.000
1728.	7.037	85.843	58.433	27.410	38.685	47364.	0.	0.	0.000
				Crystal = Liquid					
1728.	7.433	95.770	58.433	37.337	38.952	64519.	0.	0.	0.000
1750.	7.455	96.263	58.905	37.358	38.952	65376.	0.	0.	0.000
2 s	1.441	----	----	----	----	----	0.	0.	0.000
1800.	7.506	97.360	59.959	37.402	38.952	67323.	0.	0.	0.000
2 s	1.291	----	----	----	----	----	0.	0.	0.000

Table 8.17. Thermodynamic properties of bunsenite, NiO(s). The string "----" indicates that the property was not evaluated. The source of data is this study.

T	$V°$	$S°$	$-[G°_T-H°_{298}]/T$	$[H°_T-H°_{298}]/T$	$C°_p$	$H°_T-H°_{298}$	$\Delta_f H°$	$\Delta_f G°$	$\log_f K°$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	10.949	21.158	40.428	-19.270	34.098	-3854.	-240300.	-221135.	57.753
250.	10.968	29.312	37.400	-8.088	39.382	-2022.	-240374.	-216332.	45.199
2 s	0.015	0.337	0.331	0.036	0.192	9.	374.	294.	0.061
273.15	10.976	32.911	36.868	-3.958	41.923	-1081.	-240349.	-214107.	40.943
298.15	10.986	36.695	36.695	0.000	44.503	0.	-240277.	-211708.	37.090
2 s	0.015	0.331	0.331	0.000	0.168	0.	374.	278.	0.049
300.	10.987	36.971	36.696	0.277	44.687	83.	-240270.	-211530.	36.830
350.	11.008	44.212	37.258	6.954	49.263	2434.	-239992.	-206760.	30.857
400.	11.029	51.060	38.559	12.502	53.362	5001.	-239564.	-202040.	26.383
450.	11.051	57.585	40.313	17.273	57.634	7773.	-238994.	-197383.	22.911
500.	11.073	63.955	42.359	21.596	64.227	10798.	-238237.	-192797.	20.141
2 s	0.016	0.336	0.331	0.044	0.202	22.	376.	215.	0.022
519.	11.082	66.437	43.194	23.243	69.374	12063.	-237855.	-191078.	19.231
2 s	0.016	0.336	0.332	0.044	0.335	23.	376.	209.	0.021
					T_N				
519.	11.082	66.437	43.194	23.243	69.374	12063.	-237855.	-191078.	19.231
550.	11.096	69.930	44.606	25.324	56.916	13928.	-237454.	-188297.	17.883
600.	11.120	74.768	46.922	27.845	54.913	16707.	-237126.	-183844.	16.005
631.	11.134	77.529	48.359	29.170	54.754	18406.	-237053.	-181094.	14.991
					Ni(T_N)				
631.	11.134	77.529	48.359	29.170	54.754	18406.	-237052.	-181094.	14.991
650.	11.143	79.153	49.235	29.918	54.775	19447.	-236959.	-179410.	14.417
700.	11.167	83.219	51.519	31.700	54.974	22190.	-236629.	-174995.	13.058
750.	11.191	87.020	53.760	33.260	55.220	24945.	-236268.	-170606.	11.882
2 s	0.015	0.323	0.331	0.052	0.243	39.	370.	140.	0.010
800.	11.216	90.592	55.952	34.640	55.453	27712.	-235898.	-166240.	10.854
850.	11.240	93.960	58.090	35.871	55.671	30490.	-235530.	-161898.	9.949
900.	11.265	97.148	60.172	36.977	55.880	33279.	-235168.	-157577.	9.145
950.	11.290	100.175	62.198	37.977	56.090	36078.	-234815.	-153276.	8.428
1000.	11.314	103.058	64.170	38.888	56.309	38888.	-234473.	-148993.	7.782
2 s	0.016	0.296	0.323	0.105	0.444	105.	353.	80.	0.004
1050.	11.339	105.810	66.087	39.723	56.543	41709.	-234142.	-144728.	7.200
1100.	11.364	108.447	67.953	40.494	56.796	44543.	-233823.	-140477.	6.671
1150.	11.389	110.977	69.769	41.208	57.071	47389.	-233515.	-136241.	6.188
1200.	11.415	113.412	71.537	41.875	57.370	50250.	-233217.	-132018.	5.746
1250.	11.440	115.761	73.260	42.501	57.694	53126.	-232929.	-127808.	5.341
2 s	0.018	0.298	0.311	0.177	0.616	221.	359.	63.	0.003
1300.	11.465	118.030	74.938	43.092	58.045	56020.	-232650.	-123609.	4.967
1350.	11.490	120.228	76.575	43.653	58.423	58931.	-232379.	-119420.	4.621
1400.	11.516	122.360	78.172	44.188	58.829	61863.	-232114.	-115241.	4.300
1450.	11.541	124.432	79.732	44.700	59.261	64815.	-231856.	-111071.	4.001
1500.	11.566	126.449	81.256	45.193	59.719	67789.	-231602.	-106911.	3.723
2 s	0.020	0.344	0.299	0.251	0.930	376.	430.	113.	0.004
1550.	11.591	128.415	82.745	45.669	60.204	70787.	-231352.	-102759.	3.463
1600.	11.617	130.334	84.203	46.131	60.715	73810.	-231105.	-98614.	3.219
1650.	11.642	132.210	85.629	46.581	61.251	76859.	-230859.	-94478.	2.991
1700.	11.667	134.047	87.026	47.021	61.811	79935.	-230614.	-90349.	2.776
1728.	11.682	135.060	87.796	47.263	62.135	81671.	-230477.	-88040.	2.661
					-Ni(Crystal = Liquid)-				
1728.	11.682	135.060	87.796	47.263	62.135	81671.	-247631.	-88040.	2.661
1750.	11.693	135.847	88.396	47.452	62.395	83041.	-247526.	-86009.	2.567
2 s	0.024	0.450	0.293	0.350	1.484	613.	624.	196.	0.006
1800.	11.718	137.613	89.738	47.875	63.003	86175.	-247269.	-81397.	2.362
2 s	0.025	0.480	0.293	0.376	1.622	677.	683.	217.	0.006

Table 8.18. Thermodynamic properties of oxygen, $O_2(g)$. The string "----" indicates that the property was not evaluated. The source of data is Garvin and others (1987).

T	$V°$	$S°$	$\frac{-[G°_T-H°_{298}]}{T}$	$\frac{[H°_T-H°_{298}]}{T}$	$C°_p$	$H°_T-H°_{298}$	$\Delta_f H°$	$\Delta_f G°$	$\log {}_f K°$
K	cm³/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	----	193.487	207.831	-14.345	28.818	-2869.	0.	0.	0.000
250.	----	199.990	205.635	-5.644	29.276	-1411.	0.	0.	0.000
273.15	----	202.584	205.268	-2.684	29.304	-733.	0.	0.	0.000
298.15	----	205.152	205.152	0.000	29.364	0.	0.	0.	0.000
300.	----	205.334	205.153	0.180	29.371	54.	0.	0.	0.000
350.	----	209.880	205.511	4.369	29.651	1529.	0.	0.	0.000
400.	----	213.867	206.312	7.555	30.083	3022.	0.	0.	0.000
450.	----	217.439	207.353	10.087	30.588	4539.	0.	0.	0.000
500.	----	220.689	208.526	12.162	31.113	6081.	0.	0.	0.000
550.	----	223.678	209.770	13.909	31.626	7650.	0.	0.	0.000
600.	----	226.451	211.046	15.405	32.114	9243.	0.	0.	0.000
650.	----	229.040	212.331	16.709	32.568	10861.	0.	0.	0.000
700.	----	231.469	213.612	17.857	32.987	12500.	0.	0.	0.000
750.	----	233.758	214.880	18.879	33.373	14159.	0.	0.	0.000
800.	----	235.923	216.128	19.795	33.725	15836.	0.	0.	0.000
850.	----	237.978	217.353	20.625	34.049	17531.	0.	0.	0.000
900.	----	239.932	218.554	21.379	34.345	19241.	0.	0.	0.000
950.	----	241.797	219.729	22.068	34.617	20965.	0.	0.	0.000
1000.	----	243.579	220.877	22.702	34.867	22702.	0.	0.	0.000
1050.	----	245.286	221.999	23.287	35.098	24451.	0.	0.	0.000
1100.	----	246.923	223.095	23.828	35.311	26211.	0.	0.	0.000
1150.	----	248.497	224.165	24.332	35.509	27982.	0.	0.	0.000
1200.	----	250.013	225.211	24.802	35.693	29762.	0.	0.	0.000
1250.	----	251.473	226.232	25.241	35.865	31551.	0.	0.	0.000
1300.	----	252.883	227.230	25.652	36.025	33348.	0.	0.	0.000
1350.	----	254.246	228.206	26.040	36.176	35154.	0.	0.	0.000
1400.	----	255.564	229.160	26.404	36.318	36966.	0.	0.	0.000
1450.	----	256.841	230.092	26.748	36.452	38785.	0.	0.	0.000
1500.	----	258.079	231.005	27.074	36.579	40611.	0.	0.	0.000
1550.	----	259.280	231.897	27.383	36.700	42443.	0.	0.	0.000
1600.	----	260.447	232.771	27.676	36.815	44281.	0.	0.	0.000
1650.	----	261.581	233.627	27.954	36.925	46124.	0.	0.	0.000
1700.	----	262.685	234.466	28.219	37.030	47973.	0.	0.	0.000
1750.	----	263.760	235.287	28.473	37.131	49827.	0.	0.	0.000
1800.	----	264.808	236.093	28.714	37.228	51686.	0.	0.	0.000

Table 8.19. Thermodynamic properties of silicon, Si(s,l). The string "----" indicates that the property was not evaluated. The source of data is Chase and others (1985).

T	V°	S°	$-[G^\circ_T-H^\circ_{298}]/T$	$[H^\circ_T-H^\circ_{298}]/T$	C°_p	$H^\circ_T-H^\circ_{298}$	Δ_fH°	Δ_fG°	$\log {}_fK^\circ$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	----	11.648	20.521	-8.875	15.588	-1775.	0.	0.	0.000
250.	----	15.440	19.130	-3.692	18.271	-923.	0.	0.	0.000
273.15	----	17.097	18.888	-1.790	19.154	-489.	0.	0.	0.000
298.15	----	18.810	18.810	0.000	19.946	0.	0.	0.	0.000
300.	----	18.934	18.810	0.123	19.999	37.	0.	0.	0.000
350.	----	22.113	19.059	3.054	21.222	1069.	0.	0.	0.000
400.	----	25.010	19.624	5.385	22.146	2154.	0.	0.	0.000
450.	----	27.662	20.372	7.289	22.875	3280.	0.	0.	0.000
500.	----	30.104	21.225	8.878	23.470	4439.	0.	0.	0.000
550.	----	32.365	22.136	10.229	23.970	5626.	0.	0.	0.000
600.	----	34.469	23.077	11.392	24.398	6835.	0.	0.	0.000
650.	----	36.437	24.030	12.408	24.771	8065.	0.	0.	0.000
700.	----	38.285	24.983	13.303	25.100	9312.	0.	0.	0.000
750.	----	40.027	25.928	14.099	25.394	10574.	0.	0.	0.000
800.	----	41.675	26.861	14.814	25.659	11851.	0.	0.	0.000
850.	----	43.238	27.779	15.459	25.901	13140.	0.	0.	0.000
900.	----	44.724	28.680	16.044	26.122	14440.	0.	0.	0.000
950.	----	46.142	29.562	16.581	26.327	15752.	0.	0.	0.000
1000.	----	47.498	30.425	17.073	26.517	17073.	0.	0.	0.000
1050.	----	48.796	31.269	17.527	26.693	18403.	0.	0.	0.000
1100.	----	50.041	32.094	17.947	26.859	19742.	0.	0.	0.000
1150.	----	51.239	32.901	18.338	27.015	21089.	0.	0.	0.000
1200.	----	52.392	33.689	18.703	27.162	22443.	0.	0.	0.000
1250.	----	53.503	34.459	19.044	27.302	23805.	0.	0.	0.000
1300.	----	54.577	35.213	19.364	27.435	25173.	0.	0.	0.000
1350.	----	55.614	35.949	19.665	27.561	26548.	0.	0.	0.000
1400.	----	56.619	36.669	19.949	27.682	27929.	0.	0.	0.000
1450.	----	57.592	37.374	20.218	27.797	29316.	0.	0.	0.000
1500.	----	58.537	38.064	20.473	27.908	30709.	0.	0.	0.000
1550.	----	59.454	38.739	20.714	28.015	32107.	0.	0.	0.000
1600.	----	60.345	39.401	20.944	28.118	33510.	0.	0.	0.000
1650.	----	61.211	40.048	21.163	28.217	34919.	0.	0.	0.000
1685.	----	61.804	40.494	21.310	28.285	35908.	0.	0.	0.000
----------------------------------Si(Crystal = Liquid)----------------------------------									
1685.	----	91.805	40.494	51.311	25.522	86459.	0.	0.	0.000
1700.	----	92.031	40.948	51.083	25.522	86841.	0.	0.	0.000
1750.	----	92.771	42.418	50.353	25.522	88117.	0.	0.	0.000
1800.	----	93.490	43.827	49.663	25.522	89394.	0.	0.	0.000

Table 8.20. Thermodynamic properties of cristobalite ("s3=low=alpha","s4=high=beta"), SiO_2(s3,s4). The string "----" indicates that the property was not evaluated. The source of data is this study.

T	V°	S°	$\frac{-[G_T^\circ - H_{298}^\circ]}{T}$	$\frac{[H_T^\circ - H_{298}^\circ]}{T}$	C_p°	$H_T^\circ - H_{298}^\circ$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	25.509	27.867	47.145	-19.280	32.919	-3856.	-907275.	-871822.	227.692
250.	25.637	35.950	44.103	-8.152	39.586	-2038.	-907767.	-862898.	180.289
2 s	0.404	----	----	----	----	----	----	----	----
273.15	25.693	39.575	43.566	-3.990	42.269	-1090.	-907931.	-858735.	164.213
298.15	25.751	43.392	43.392	0.000	44.897	0.	-908063.	-854226.	149.654
2 s	0.186	----	----	----	----	----	----	----	----
300.	25.755	43.671	43.393	0.277	45.081	83.	-908071.	-853892.	148.673
350.	25.865	50.968	43.959	7.009	49.562	2453.	-908208.	-844849.	126.084
400.	25.967	57.834	45.269	12.565	53.237	5026.	-908213.	-835796.	109.141
450.	26.063	64.285	47.027	17.258	56.278	7766.	-908116.	-826749.	95.965
500.	26.153	70.350	49.059	21.290	58.816	10645.	-907938.	-817717.	85.425
2 s	0.094	----	----	----	----	----	----	----	----
543.	26.227	75.280	50.942	24.337	60.672	13215.	-907735.	-809966.	77.914
(alpha) = (beta)									
543.	27.264	77.724	50.942	26.783	59.421	14543.	-906407.	-809966.	77.914
550.	27.270	78.487	51.288	27.200	59.785	14960.	-906379.	-808723.	76.805
600.	27.309	83.790	53.777	30.013	62.037	18008.	-906134.	-799856.	69.632
650.	27.342	88.828	56.281	32.546	63.804	21155.	-905833.	-791011.	63.565
700.	27.370	93.610	58.778	34.831	65.220	24382.	-905492.	-782191.	58.367
750.	27.393	98.151	61.253	36.897	66.374	27673.	-905123.	-773397.	53.863
2 s	0.034	----	----	----	----	----	----	----	----
800.	27.413	102.466	63.695	38.770	67.331	31016.	-904733.	-764628.	49.924
850.	27.430	106.572	66.098	40.475	68.134	34404.	-904330.	-755883.	46.450
900.	27.444	110.487	68.456	42.031	68.818	37828.	-903916.	-747163.	43.363
950.	27.456	114.224	70.767	43.457	69.407	41284.	-903496.	-738466.	40.603
1000.	27.466	117.797	73.030	44.767	69.919	44767.	-903070.	-729791.	38.120
2 s	0.045	----	----	----	----	----	----	----	----
1050.	27.475	121.220	75.244	45.976	70.369	48275.	-902643.	-721138.	35.874
1100.	27.482	124.503	77.409	47.094	70.768	51803.	-902213.	-712505.	33.833
1150.	27.489	127.656	79.525	48.131	71.123	55351.	-901783.	-703891.	31.971
1200.	27.494	130.690	81.594	49.096	71.444	58915.	-901353.	-695297.	30.265
1207.45	27.494	131.133	81.899	49.234	71.489	59448.	-901289.	-694017.	30.023
-Quartz(beta) = Cristobalite(beta)-									
1207.45	27.494	131.133	81.899	49.234	71.489	59448.	-901289.	-694017.	30.023
1250.	27.498	133.613	83.617	49.996	71.734	62495.	-900924.	-686720.	28.696
2 s	0.054	----	----	----	----	----	----	----	----
1300.	27.502	136.431	85.594	50.837	71.998	66088.	-900497.	-678160.	27.248
1350.	27.505	139.153	87.528	51.625	72.241	69694.	-900071.	-669617.	25.908
1400.	27.508	141.785	89.419	52.366	72.465	73312.	-899647.	-661089.	24.665
1450.	27.510	144.331	91.269	53.062	72.673	76940.	-899224.	-652577.	23.508
1500.	27.512	146.798	93.079	53.719	72.867	80579.	-898804.	-644079.	22.428
2 s	0.059	----	----	----	----	----	----	----	----
1550.	27.514	149.190	94.851	54.340	73.048	84227.	-898386.	-635595.	21.419
1600.	27.515	151.512	96.585	54.928	73.219	87884.	-897971.	-627124.	20.473
1650.	27.516	153.768	98.284	55.484	73.380	91549.	-897558.	-618667.	19.585
1685.	27.517	155.309	99.452	55.857	73.488	94119.	-897270.	-612754.	18.995
-Si(Crystal = Liquid)-									
1685.	27.517	155.309	99.452	55.857	73.488	94119.	-947821.	-612754.	18.995
1700.	27.517	155.961	99.948	56.012	73.533	95221.	-947656.	-609772.	18.736
1750.	27.518	158.094	101.579	56.515	73.678	98902.	-947106.	-599842.	17.904
2 s	0.060	----	----	----	----	----	----	----	----
1800.	27.519	160.172	103.178	56.994	73.816	102589.	-946554.	-589928.	17.119
2 s	0.061	----	----	----	----	----	----	----	----

Table 8.21. Thermodynamic properties of quartz ("s1=low=alpha","s2=high=beta"), SiO_2(s1,s2). The string "----" indicates that the property was not evaluated. The source of data is this study.

T	V°	S°	$-[G^\circ_T-H^\circ_{298}]/T$	$[H^\circ_T-H^\circ_{298}]/T$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log $_fK^\circ$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	22.631	26.046	45.177	-19.130	32.649	-3826.	-909885.	-874067.	228.278
250.	22.663	34.067	42.158	-8.092	39.279	-2023.	-910391.	-865050.	180.739
2 s	0.071	----	----	----	----	----	----	----	----
273.15	22.680	37.664	41.625	-3.961	41.946	-1082.	-910562.	-860844.	164.616
298.15	22.701	41.453	41.453	0.000	44.586	0.	-910702.	-856287.	150.015
2 s	0.052	----	----	----	----	----	----	----	----
300.	22.702	41.729	41.453	0.277	44.773	83.	-910710.	-855949.	149.031
350.	22.747	48.988	42.016	6.971	49.403	2440.	-910860.	-846808.	126.377
400.	22.797	55.851	43.321	12.530	53.378	5012.	-910866.	-837656.	109.384
450.	22.852	62.342	45.077	17.264	56.837	7769.	-910752.	-828510.	96.169
500.	22.909	68.491	47.113	21.378	59.880	10689.	-910534.	-819383.	85.599
2 s	0.041	----	----	----	----	----	----	----	----
550.	22.970	74.327	49.324	25.004	62.580	13752.	-910226.	-810282.	76.953
600.	23.034	79.878	51.641	28.237	64.990	16942.	-909838.	-801213.	69.750
650.	23.100	85.167	54.018	31.149	67.154	20247.	-909381.	-792179.	63.659
700.	23.167	90.216	56.425	33.791	69.104	23654.	-908859.	-783183.	58.441
750.	23.236	95.045	58.840	36.205	70.868	27154.	-908281.	-774225.	53.921
2 s	0.040	----	----	----	----	----	----	----	----
800.	23.307	99.670	61.248	38.423	72.467	30738.	-907651.	-765309.	49.968
845.5	23.372	103.716	63.425	40.291	73.796	34066.	-907037.	-757230.	46.780
(alpha) = (beta)									
845.5	23.668	104.767	63.425	41.341	68.716	34954.	-906148.	-757230.	46.780
850.	23.669	105.131	63.645	41.486	68.702	35263.	-906109.	-756438.	46.484
900.	23.683	109.056	66.060	42.996	68.635	38696.	-905687.	-747646.	43.391
950.	23.695	112.768	68.421	44.346	68.701	42129.	-905289.	-738877.	40.625
1000.	23.705	116.296	70.728	45.568	68.869	45568.	-904909.	-730128.	38.137
2 s	0.038	----	----	----	----	----	----	----	----
1050.	23.714	119.661	72.978	46.683	69.118	49017.	-904539.	-721398.	35.887
1100.	23.721	122.884	75.174	47.710	69.430	52481.	-904174.	-712686.	33.842
1150.	23.727	125.978	77.316	48.662	69.793	55961.	-903812.	-703990.	31.976
1200.	23.732	128.957	79.406	49.551	70.195	59461.	-903447.	-695309.	30.265
1207.45	23.733	129.391	79.713	49.678	70.258	59984.	-903392.	-694017.	30.023
-Quartz(beta) = Cristobalite(beta)-									
1207.45	23.733	129.391	79.713	49.678	70.258	59984.	-903392.	-694017.	30.023
1250.	23.737	131.831	81.446	50.385	70.631	62981.	-903077.	-686645.	28.693
2 s	0.058	----	----	----	----	----	----	----	----
1300.	23.740	134.610	83.438	51.172	71.092	66524.	-902699.	-677995.	27.242
1350.	23.744	137.302	85.383	51.919	71.573	70091.	-902313.	-669360.	25.899
1400.	23.746	139.914	87.284	52.630	72.072	73682.	-901915.	-660739.	24.652
1450.	23.749	142.452	89.143	53.309	72.584	77298.	-901505.	-652133.	23.492
1500.	23.751	144.921	90.961	53.960	73.107	80940.	-901082.	-643541.	22.410
2 s	0.071	----	----	----	----	----	----	----	----
1550.	23.752	147.327	92.741	54.586	73.639	84609.	-900643.	-634963.	21.398
1600.	23.753	149.674	94.483	55.190	74.177	88304.	-900189.	-626400.	20.449
1650.	23.755	151.964	96.191	55.774	74.721	92027.	-899718.	-617852.	19.559
1685.	23.755	153.537	97.366	56.172	75.105	94649.	-899379.	-611876.	18.968
-Si(Crystal = Liquid)-									
1685.	23.755	153.537	97.366	56.172	75.105	94649.	-949930.	-611876.	18.968
1700.	23.756	154.203	97.864	56.339	75.270	95777.	-949740.	-608868.	18.708
1750.	23.756	156.393	99.505	56.888	75.821	99554.	-949093.	-598851.	17.874
2 s	0.077	----	----	----	----	----	----	----	----
1800.	23.757	158.537	101.115	57.422	76.376	103359.	-948423.	-588854.	17.088
2 s	0.078	----	----	----	----	----	----	----	----

Table 9.01. Composition of wustite at the iron-wustite boundary, the activities of Fe, FeO, and O_2, and the equilibrium constant for the reaction "2 Fe(s) + O_2(g) = 2 FeO(wus,sln)". Values in parentheses are for the metastable extensions.

Temperature (K)	y	x	log a(Fe)	log a(FeO)	log a(O_2)	log $_rK°$
	------moles------					
800.	(0.0915)	(0.1008)	(0.0000)	(-0.0530)	(-27.6476)	(27.5416)
825.	(0.0859)	(0.0940)	(0.0000)	(-0.0464)	(-26.6064)	(26.5137)
839.15	0.0830	0.0905	0.0000	-0.0431	-26.0451	25.9589
850.	0.0809	0.0880	0.0000	-0.0408	-25.6276	25.5459
875.	0.0763	0.0826	0.0000	-0.0362	-24.7055	24.6332
900.	0.0722	0.0778	0.0000	-0.0322	-23.8352	23.7707
925.	0.0684	0.0735	0.0000	-0.0289	-23.0122	22.9543
950.	0.0651	0.0697	0.0000	-0.0261	-22.2325	22.1803
1000.	0.0595	0.0633	0.0000	-0.0218	-20.7894	20.7458
1050.	0.0551	0.0583	0.0000	-0.0187	-19.4806	19.4432
1100.	0.0517	0.0545	0.0000	-0.0165	-18.2875	18.2545
1150.	0.0492	0.0517	0.0000	-0.0150	-17.1974	17.1674
1184.	0.0479	0.0503	0.0000	-0.0143	-16.5086	16.4801
			Fe(α)=Fe(γ)			
1184.	0.0479	0.0503	0.0000	-0.0143	-16.5086	16.4801
1200.	0.0475	0.0499	0.0000	-0.0141	-16.1972	16.1691
1250.	0.0465	0.0488	0.0000	-0.0136	-15.2760	15.2488
1300.	0.0460	0.0482	0.0000	-0.0134	-14.4269	14.4000
1350.	0.0458	0.0480	0.0000	-0.0134	-13.6416	13.6147
1400.	0.0460	0.0482	0.0000	-0.0137	-12.9133	12.8860
1450.	0.0464	0.0487	0.0000	-0.0141	-12.2360	12.2079
1500.	0.0471	0.0494	0.0000	-0.0146	-11.6047	11.5755
1550.	0.0479	0.0503	0.0000	-0.0153	-11.0148	10.9843
1600.	0.0489	0.0514	0.0000	-0.0161	-10.4625	10.4303
1645.	0.0499	0.0525	0.0000	-0.0169	-9.9947	9.9608
1650.	(0.0500)	(0.0526)	(0.0000)	(-0.0170)	(-9.9443)	(9.9103)
1665.	(0.0503)	(0.0530)	(0.0000)	(-0.0173)	(-9.7950)	(9.7604)
			Fe(γ)=Fe(α)			
1665.	(0.0503)	(0.0530)	(0.0000)	(-0.0173)	(-9.7950)	(9.7604)
1697.15	(0.0512)	(0.0540)	(0.0000)	(-0.0181)	(-9.4833)	(9.4471)
1700.	(0.0513)	(0.0541)	(0.0000)	(-0.0181)	(-9.4562)	(9.4199)

Table 9.02. Composition of wustite at the wustite-magnetite boundary, the activities of Fe, FeO, and O_2, and the equilibrium constant for the reaction "6 FeO(wus,sln) + O_2(g) = 2 Fe_3O_4(magnetite)". The values in parentheses are for the metastable extensions.

Temperature (K)	y	x	log a(Fe)	log a(FeO)	log a(O_2)	log $_rK°$
	------moles------					
800.	(0.0787)	(0.0854)	(0.1749)	(-0.0381)	(-27.9823)	(28.2110)
825.	(0.0815)	(0.0887)	(0.0608)	(-0.0413)	(-26.7217)	(26.9694)
839.15	0.0830	0.0905	0.0000	-0.0431	-26.0452	26.3039
850.	0.0842	0.0919	-0.0449	-0.0445	-25.5440	25.8112
875.	0.0868	0.0950	-0.1433	-0.0478	-24.4414	24.7285
900.	0.0893	0.0980	-0.2351	-0.0512	-23.4035	23.7109
925.	0.0918	0.1010	-0.3211	-0.0547	-22.4235	22.7516
950.	0.0942	0.1040	-0.4017	-0.0582	-21.4961	21.8454
1000.	0.0989	0.1098	-0.5496	-0.0655	-19.7815	20.1747
1050.	0.1035	0.1155	-0.6826	-0.0732	-18.2298	18.6693
1100.	0.1080	0.1211	-0.8039	-0.0814	-16.8173	17.3057
1150.	0.1125	0.1268	-0.9160	-0.0900	-15.5246	16.0649
1184.	0.1155	0.1306	-0.9881	-0.0962	-14.7057	15.2832
			Fe(α)=Fe(γ)			
1184.	0.1155	0.1306	-0.9881	-0.0962	-14.7057	15.2832
1200.	0.1170	0.1324	-1.0200	-0.0993	-14.3356	14.9312
1250.	0.1214	0.1382	-1.1171	-0.1091	-13.2369	13.8915
1300.	0.1259	0.1440	-1.2116	-0.1196	-12.2168	12.9347
1350.	0.1304	0.1499	-1.3044	-0.1309	-11.2658	12.0514
1400.	0.1349	0.1560	-1.3966	-0.1431	-10.3753	11.2336
1450.	0.1395	0.1622	-1.4889	-0.1560	-9.5381	10.4744
1500.	0.1442	0.1685	-1.5820	-0.1700	-8.7478	9.7678
1550.	0.1489	0.1749	-1.6763	-0.1849	-7.9989	9.1085
1600.	0.1536	0.1815	-1.7724	-0.2010	-7.2863	8.4921
1645.	0.1580	0.1876	-1.8609	-0.2164	-6.6725	7.9707
1650.	0.1584	0.1883	-1.8708	-0.2181	-6.6058	7.9146
1665.	0.1599	0.1903	-1.9008	-0.2235	-6.4073	7.7484
			Fe(α)=Fe(γ)			
1665.	0.1599	0.1903	-1.9008	-0.2235	-6.4073	7.7484
1697.15	0.1630	0.1948	-1.9648	-0.2354	-5.9900	7.4024
1700.	(0.1633)	(0.1952)	(-1.9705)	(-0.2365)	(-5.9535)	(7.3724)

Table 9.03. Molar volume, V°(cm^3/mol), of wustite, $Fe_{1-y}O$ for $y = 0$ to $y = 0.16$ between 200 and 1700 K at one bar total pressure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the molar volume for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y"								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
200.	(12.225)	(12.189)	(12.154)	(12.119)	(12.083)	(12.048)	(12.013)	(11.978)	(11.943)
250.	(12.226)	(12.191)	(12.156)	(12.120)	(12.085)	(12.050)	(12.015)	(11.980)	(11.945)
273.15	(12.229)	(12.193)	(12.158)	(12.123)	(12.088)	(12.052)	(12.017)	(11.982)	(11.948)
298.15	(12.232)	(12.197)	(12.162)	(12.126)	(12.091)	(12.056)	(12.021)	(11.986)	(11.951)
300.	(12.233)	(12.197)	(12.162)	(12.127)	(12.091)	(12.056)	(12.021)	(11.986)	(11.951)
350.	(12.243)	(12.207)	(12.172)	(12.137)	(12.102)	(12.066)	(12.031)	(11.996)	(11.962)
400.	(12.256)	(12.221)	(12.185)	(12.150)	(12.115)	(12.080)	(12.045)	(12.010)	(11.975)
450.	(12.272)	(12.237)	(12.201)	(12.166)	(12.131)	(12.096)	(12.061)	(12.026)	(11.991)
500.	(12.290)	(12.255)	(12.220)	(12.184)	(12.149)	(12.114)	(12.079)	(12.044)	(12.009)
550.	(12.311)	(12.275)	(12.240)	(12.205)	(12.169)	(12.134)	(12.099)	(12.064)	(12.029)
600.	(12.333)	(12.297)	(12.262)	(12.226)	(12.191)	(12.156)	(12.121)	(12.086)	(12.051)
650.	(12.356)	(12.320)	(12.285)	(12.250)	(12.215)	(12.179)	(12.144)	(12.109)	(12.075)
700.	(12.380)	(12.345)	(12.310)	(12.274)	(12.239)	(12.204)	(12.169)	(12.134)	(12.099)
750.	(12.406)	(12.370)	(12.335)	(12.300)	(12.264)	(12.229)	(12.194)	(12.159)	(12.124)
800.	(12.432)	(12.397)	(12.361)	(12.326)	(12.291)	(12.256)	(12.221)	(12.186)	(12.151)
825.	(12.446)	(12.410)	(12.375)	(12.339)	(12.304)	(12.269)	(12.234)	(12.199)	(12.164)
839.15	(12.453)	(12.418)	(12.382)	(12.347)	(12.312)	(12.277)	(12.242)	(12.207)	(12.172)
850.	(12.459)	(12.424)	(12.388)	(12.353)	(12.318)	(12.283)	(12.248)	(12.213)	(12.178)
875.	(12.473)	(12.438)	(12.402)	(12.367)	(12.332)	(12.296)	(12.262)	(12.226)	12.192
900.	(12.487)	(12.451)	(12.416)	(12.381)	(12.345)	(12.310)	(12.275)	(12.240)	12.205
925.	(12.501)	(12.465)	(12.430)	(12.395)	(12.360)	(12.324)	(12.289)	12.254	12.220
950.	(12.515)	(12.480)	(12.444)	(12.409)	(12.374)	(12.339)	(12.304)	12.268	12.234
1000.	(12.544)	(12.508)	(12.473)	(12.438)	(12.402)	(12.367)	12.332	12.297	12.262
1050.	(12.573)	(12.537)	(12.502)	(12.466)	(12.431)	(12.396)	12.361	12.326	12.291
1100.	(12.602)	(12.566)	(12.531)	(12.496)	(12.461)	(12.425)	12.390	12.355	12.320
1150.	(12.631)	(12.596)	(12.561)	(12.525)	(12.490)	12.455	12.420	12.385	12.350
1184.	(12.651)	(12.616)	(12.581)	(12.546)	(12.510)	12.475	12.440	12.405	12.370
1184.	(12.651)	(12.616)	(12.581)	(12.546)	(12.510)	12.475	12.440	12.405	12.370
1200.	(12.661)	(12.626)	(12.590)	(12.555)	(12.520)	12.485	12.450	12.415	12.380
1250.	(12.691)	(12.656)	(12.620)	(12.585)	(12.550)	12.515	12.480	12.445	12.410
1300.	(12.721)	(12.686)	(12.650)	(12.615)	(12.580)	12.545	12.510	12.475	12.440
1350.	(12.751)	(12.716)	(12.681)	(12.645)	(12.610)	12.575	12.540	12.505	12.470
1400.	(12.782)	(12.746)	(12.711)	(12.676)	(12.641)	12.605	12.570	12.535	12.500
1450.	(12.812)	(12.777)	(12.742)	(12.706)	(12.671)	12.636	12.601	12.566	12.531
1500.	(12.843)	(12.807)	(12.772)	(12.737)	(12.702)	12.666	12.631	12.596	12.561
1550.	(12.873)	(12.838)	(12.803)	(12.767)	(12.732)	12.697	12.662	12.627	12.592
1600.	(12.904)	(12.869)	(12.833)	(12.798)	(12.763)	12.728	12.693	12.658	12.623
1645.	(12.932)	(12.896)	(12.861)	(12.826)	(12.790)	12.755	12.720	12.685	12.650
1650.	(12.935)	(12.899)	(12.864)	(12.829)	(12.794)	(12.758)	(12.723)	12.688	12.653
1665.	(12.944)	(12.909)	(12.873)	(12.838)	(12.803)	(12.768)	(12.733)	(12.698)	(12.663)
1665.	(12.944)	(12.909)	(12.873)	(12.838)	(12.803)	(12.768)	(12.733)	(12.698)	(12.663)
1697.15	(12.964)	(12.928)	(12.893)	(12.858)	(12.823)	(12.787)	(12.752)	(12.717)	(12.683)
1700.	(12.966)	(12.930)	(12.895)	(12.859)	(12.824)	(12.789)	(12.754)	(12.719)	(12.684)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

Table 9.03 Continued. Molar volume, $V°(cm^3/mol)$, of wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite as "y"								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
200.	(11.943)	(11.909)	(11.874)	(11.839)	(11.804)	(11.770)	(11.735)	(11.701)	(11.666)
250.	(11.945)	(11.910)	(11.875)	(11.841)	(11.806)	(11.772)	(11.737)	(11.702)	(11.668)
273.15	(11.948)	(11.913)	(11.878)	(11.843)	(11.808)	(11.774)	(11.739)	(11.705)	(11.671)
298.15	(11.951)	(11.916)	(11.881)	(11.847)	(11.812)	(11.778)	(11.743)	(11.708)	(11.674)
300.	(11.951)	(11.917)	(11.882)	(11.847)	(11.812)	(11.778)	(11.743)	(11.709)	(11.674)
350.	(11.962)	(11.927)	(11.892)	(11.857)	(11.822)	(11.788)	(11.753)	(11.719)	(11.685)
400.	(11.975)	(11.940)	(11.905)	(11.870)	(11.836)	(11.801)	(11.767)	(11.732)	(11.698)
450.	(11.991)	(11.956)	(11.921)	(11.886)	(11.852)	(11.817)	(11.783)	(11.748)	(11.714)
500.	(12.009)	(11.974)	(11.939)	(11.905)	(11.870)	(11.835)	(11.801)	(11.766)	(11.732)
550.	(12.029)	(11.994)	(11.960)	(11.925)	(11.890)	(11.856)	(11.821)	(11.787)	(11.752)
600.	(12.051)	(12.016)	(11.982)	(11.947)	(11.912)	(11.878)	(11.843)	(11.809)	(11.774)
650.	(12.075)	(12.040)	(12.005)	(11.970)	(11.935)	(11.901)	(11.866)	(11.832)	(11.798)
700.	(12.099)	(12.064)	(12.029)	(11.995)	(11.960)	(11.925)	(11.891)	(11.856)	(11.822)
750.	(12.124)	(12.090)	(12.055)	(12.020)	(11.985)	(11.951)	(11.916)	(11.882)	(11.847)
800.	(12.151)	(12.116)	(12.081)	(12.046)	(12.012)	(11.977)	(11.943)	(11.908)	(11.874)
825.	(12.164)	(12.129)	(12.095)	(12.060)	(12.025)	(11.991)	(11.956)	(11.922)	(11.887)
839.15	(12.172)	(12.137)	(12.102)	(12.067)	(12.033)	(11.998)	(11.964)	(11.929)	(11.895)
850.	(12.178)	(12.143)	(12.108)	(12.073)	(12.039)	(12.004)	(11.970)	(11.935)	(11.901)
875.	12.192	(12.157)	(12.122)	(12.087)	(12.052)	(12.018)	(11.983)	(11.949)	(11.915)
900.	12.205	(12.171)	(12.136)	(12.101)	(12.066)	(12.032)	(11.997)	(11.963)	(11.929)
925.	12.220	12.185	(12.150)	(12.115)	(12.080)	(12.046)	(12.011)	(11.977)	(11.942)
950.	12.234	12.199	(12.164)	(12.129)	(12.095)	(12.060)	(12.026)	(11.991)	(11.957)
1000.	12.262	12.227	(12.192)	(12.158)	(12.123)	(12.089)	(12.054)	(12.020)	(11.985)
1050.	12.291	12.256	12.222	(12.187)	(12.152)	(12.117)	(12.083)	(12.049)	(12.014)
1100.	12.320	12.286	12.251	(12.216)	(12.181)	(12.147)	(12.112)	(12.078)	(12.044)
1150.	12.350	12.315	12.280	12.246	(12.211)	(12.176)	(12.142)	(12.107)	(12.073)
1184.	12.370	12.335	12.301	12.266	(12.231)	(12.197)	(12.162)	(12.128)	(12.093)
1184.	12.370	12.335	12.301	12.266	(12.231)	(12.197)	(12.162)	(12.128)	(12.093)
1200.	12.380	12.345	12.310	12.275	(12.241)	(12.206)	(12.172)	(12.137)	(12.103)
1250.	12.410	12.375	12.340	12.305	12.271	(12.236)	(12.202)	(12.167)	(12.133)
1300.	12.440	12.405	12.370	12.335	12.301	(12.266)	(12.232)	(12.197)	(12.163)
1350.	12.470	12.435	12.400	12.366	12.331	12.296	(12.262)	(12.228)	(12.193)
1400.	12.500	12.466	12.431	12.396	12.361	12.327	(12.292)	(12.258)	(12.224)
1450.	12.531	12.496	12.461	12.427	12.392	12.357	(12.323)	(12.288)	(12.254)
1500.	12.561	12.527	12.492	12.457	12.422	12.388	12.353	(12.319)	(12.284)
1550.	12.592	12.557	12.522	12.488	12.453	12.418	12.384	(12.349)	(12.315)
1600.	12.623	12.588	12.553	12.518	12.484	12.449	12.415	12.380	12.346
1645.	12.650	12.615	12.581	12.546	12.511	12.477	12.442	12.408	12.373
1650.	12.653	12.619	12.584	12.549	12.514	12.480	12.445	12.411	12.377
1665.	(12.663)	(12.628)	12.593	12.558	12.524	12.489	12.454	12.420	12.386
1665.	(12.663)	(12.628)	12.593	12.558	12.524	12.489	12.454	12.420	12.386
1697.15	(12.683)	(12.648)	(12.613)	(12.578)	(12.543)	(12.509)	(12.474)	(12.440)	(12.405)
1700.	(12.684)	(12.649)	(12.615)	(12.580)	(12.545)	(12.511)	(12.476)	(12.442)	(12.407)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.04. Molar heat capacity, Cp° [J/mol K)], of wustite, $Fe_{1-y}O$ for y = 0 to y = 0.16 between 200 and 1700 K at one bar total pressure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the molar heat capacity for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
200.	(45.143)	(45.375)	(45.606)	(45.834)	(46.061)	(46.286)	(46.509)	(46.730)	(46.949)
250.	(45.301)	(45.541)	(45.778)	(46.013)	(46.246)	(46.476)	(46.704)	(46.930)	(47.152)
273.15	(46.478)	(46.709)	(46.937)	(47.163)	(47.387)	(47.608)	(47.826)	(48.042)	(48.254)
298.15	(47.529)	(47.753)	(47.974)	(48.193)	(48.409)	(48.622)	(48.832)	(49.040)	(49.244)
300.	(47.598)	(47.822)	(48.043)	(48.261)	(48.476)	(48.689)	(48.899)	(49.105)	(49.309)
350.	(49.095)	(49.311)	(49.525)	(49.735)	(49.942)	(50.146)	(50.347)	(50.543)	(50.737)
400.	(50.097)	(50.312)	(50.524)	(50.732)	(50.937)	(51.137)	(51.334)	(51.527)	(51.716)
450.	(50.813)	(51.030)	(51.244)	(51.453)	(51.658)	(51.859)	(52.055)	(52.247)	(52.434)
500.	(51.360)	(51.581)	(51.798)	(52.010)	(52.218)	(52.420)	(52.618)	(52.811)	(52.999)
550.	(51.806)	(52.031)	(52.252)	(52.468)	(52.679)	(52.885)	(53.085)	(53.280)	(53.469)
600.	(52.189)	(52.420)	(52.646)	(52.866)	(53.081)	(53.290)	(53.493)	(53.690)	(53.881)
650.	(52.535)	(52.771)	(53.002)	(53.227)	(53.446)	(53.658)	(53.865)	(54.064)	(54.257)
700.	(52.859)	(53.101)	(53.337)	(53.566)	(53.789)	(54.005)	(54.215)	(54.417)	(54.612)
750.	(53.171)	(53.418)	(53.659)	(53.893)	(54.120)	(54.339)	(54.552)	(54.757)	(54.954)
800.	(53.476)	(53.729)	(53.974)	(54.213)	(54.444)	(54.667)	(54.883)	(55.090)	(55.289)
825.	(53.629)	(53.884)	(54.131)	(54.372)	(54.605)	(54.830)	(55.047)	(55.255)	(55.455)
839.15	(53.715)	(53.971)	(54.220)	(54.462)	(54.696)	(54.922)	(55.140)	(55.349)	(55.550)
850.	(53.781)	(54.038)	(54.288)	(54.531)	(54.766)	(54.993)	(55.211)	(55.421)	(55.622)
875.	(53.933)	(54.193)	(54.446)	(54.690)	(54.927)	(55.155)	(55.375)	(55.586)	55.788
900.	(54.086)	(54.348)	(54.603)	(54.850)	(55.088)	(55.318)	(55.539)	(55.751)	55.954
925.	(54.239)	(54.504)	(54.761)	(55.010)	(55.250)	(55.482)	(55.704)	55.917	56.120
950.	(54.394)	(54.661)	(54.920)	(55.171)	(55.413)	(55.646)	(55.870)	56.084	56.288
1000.	(54.705)	(54.977)	(55.241)	(55.496)	(55.741)	(55.977)	56.203	56.419	56.624
1050.	(55.021)	(55.298)	(55.566)	(55.824)	(56.073)	(56.312)	56.540	56.758	56.964
1100.	(55.343)	(55.624)	(55.896)	(56.158)	(56.409)	(56.651)	56.881	57.100	57.308
1150.	(55.669)	(55.955)	(56.230)	(56.496)	(56.750)	56.994	57.226	57.447	57.656
1184.	(55.894)	(56.183)	(56.461)	(56.728)	(56.985)	57.230	57.464	57.686	57.895
1184.	(55.894)	(56.183)	(56.461)	(56.728)	(56.985)	57.230	57.464	57.686	57.895
1200.	(56.001)	(56.290)	(56.570)	(56.838)	(57.096)	57.342	57.577	57.799	58.008
1250.	(56.338)	(56.631)	(56.915)	(57.186)	(57.447)	57.695	57.931	58.154	58.365
1300.	(56.679)	(56.977)	(57.264)	(57.539)	(57.802)	58.052	58.290	58.515	58.726
1350.	(57.026)	(57.328)	(57.618)	(57.896)	(58.162)	58.414	58.653	58.879	59.091
1400.	(57.378)	(57.684)	(57.977)	(58.258)	(58.526)	58.780	59.021	59.248	59.460
1450.	(57.734)	(58.044)	(58.340)	(58.624)	(58.894)	59.151	59.393	59.620	59.833
1500.	(58.095)	(58.408)	(58.708)	(58.994)	(59.267)	59.525	59.768	59.997	60.209
1550.	(58.460)	(58.777)	(59.079)	(59.369)	(59.643)	59.903	60.148	60.377	60.590
1600.	(58.829)	(59.149)	(59.455)	(59.747)	(60.024)	60.285	60.531	60.761	60.974
1645.	(59.165)	(59.488)	(59.796)	(60.090)	(60.369)	60.632	60.879	61.109	61.322
1650.	(59.202)	(59.525)	(59.834)	(60.128)	(60.407)	(60.671)	(60.918)	61.148	61.361
1665.	(59.315)	(59.639)	(59.949)	(60.244)	(60.523)	(60.787)	(61.034)	(61.265)	(61.478)
1665.	(59.315)	(59.639)	(59.949)	(60.244)	(60.523)	(60.787)	(61.034)	(61.265)	(61.478)
1697.15	(59.557)	(59.884)	(60.195)	(60.492)	(60.773)	(61.037)	(61.285)	(61.516)	(61.729)
1700.	(59.579)	(59.905)	(60.217)	(60.514)	(60.795)	(61.059)	(61.308)	(61.538)	(61.751)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

Table 9.04 Continued. Molar heat capacity, $C_p°$ [J/mol K)], of wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
200.	(46.949)	(47.165)	(47.380)	(47.592)	(47.802)	(48.009)	(48.213)	(48.415)	(48.615)
250.	(47.152)	(47.372)	(47.590)	(47.804)	(48.016)	(48.224)	(48.429)	(48.631)	(48.829)
273.15	(48.254)	(48.464)	(48.671)	(48.874)	(49.074)	(49.271)	(49.465)	(49.654)	(49.840)
298.15	(49.244)	(49.444)	(49.642)	(49.836)	(50.027)	(50.213)	(50.396)	(50.575)	(50.750)
300.	(49.309)	(49.509)	(49.706)	(49.899)	(50.089)	(50.276)	(50.458)	(50.636)	(50.810)
350.	(50.737)	(50.926)	(51.112)	(51.293)	(51.470)	(51.643)	(51.812)	(51.976)	(52.135)
400.	(51.716)	(51.900)	(52.080)	(52.255)	(52.425)	(52.591)	(52.751)	(52.906)	(53.056)
450.	(52.434)	(52.617)	(52.794)	(52.966)	(53.133)	(53.294)	(53.450)	(53.599)	(53.742)
500.	(52.999)	(53.181)	(53.358)	(53.528)	(53.693)	(53.852)	(54.004)	(54.150)	(54.289)
550.	(53.469)	(53.652)	(53.829)	(53.999)	(54.163)	(54.320)	(54.471)	(54.613)	(54.749)
600.	(53.881)	(54.065)	(54.243)	(54.414)	(54.577)	(54.733)	(54.882)	(55.022)	(55.154)
650.	(54.257)	(54.443)	(54.622)	(54.793)	(54.956)	(55.111)	(55.258)	(55.397)	(55.526)
700.	(54.612)	(54.799)	(54.979)	(55.150)	(55.314)	(55.468)	(55.614)	(55.750)	(55.877)
750.	(54.954)	(55.143)	(55.323)	(55.495)	(55.658)	(55.812)	(55.956)	(56.090)	(56.214)
800.	(55.289)	(55.479)	(55.661)	(55.833)	(55.996)	(56.148)	(56.291)	(56.423)	(56.544)
825.	(55.455)	(55.646)	(55.828)	(56.000)	(56.163)	(56.315)	(56.457)	(56.588)	(56.707)
839.15	(55.550)	(55.741)	(55.923)	(56.095)	(56.257)	(56.409)	(56.551)	(56.681)	(56.799)
850.	(55.622)	(55.813)	(55.995)	(56.168)	(56.330)	(56.481)	(56.622)	(56.752)	(56.870)
875.	55.788	(55.980)	(56.162)	(56.335)	(56.497)	(56.647)	(56.787)	(56.916)	(57.032)
900.	55.954	(56.147)	(56.329)	(56.502)	(56.663)	(56.814)	(56.953)	(57.080)	(57.194)
925.	56.120	56.314	(56.497)	(56.669)	(56.830)	(56.980)	(57.118)	(57.244)	(57.357)
950.	56.288	56.481	(56.665)	(56.837)	(56.998)	(57.147)	(57.284)	(57.408)	(57.519)
1000.	56.624	56.819	(57.002)	(57.174)	(57.334)	(57.482)	(57.617)	(57.738)	(57.846)
1050.	56.964	57.160	57.343	(57.515)	(57.673)	(57.819)	(57.952)	(58.071)	(58.175)
1100.	57.308	57.504	57.688	(57.858)	(58.016)	(58.160)	(58.290)	(58.406)	(58.506)
1150.	57.656	57.852	58.036	58.206	(58.362)	(58.505)	(58.632)	(58.745)	(58.841)
1184.	57.895	58.092	58.275	58.445	(58.600)	(58.741)	(58.867)	(58.977)	(59.071)
1184.	57.895	58.092	58.275	58.445	(58.600)	(58.741)	(58.867)	(58.977)	(59.071)
1200.	58.008	58.205	58.388	58.558	(58.713)	(58.853)	(58.978)	(59.087)	(59.179)
1250.	58.365	58.562	58.745	58.913	59.066	(59.205)	(59.327)	(59.432)	(59.520)
1300.	58.726	58.923	59.105	59.272	59.424	(59.560)	(59.679)	(59.781)	(59.865)
1350.	59.091	59.287	59.469	59.636	59.786	59.919	(60.035)	(60.133)	(60.213)
1400.	59.460	59.657	59.838	60.003	60.151	60.282	(60.395)	(60.489)	(60.565)
1450.	59.833	60.029	60.210	60.373	60.520	60.648	(60.758)	(60.849)	(60.920)
1500.	60.209	60.406	60.585	60.748	60.892	61.018	61.124	(61.211)	(61.277)
1550.	60.590	60.786	60.965	61.125	61.268	61.391	61.494	(61.577)	(61.638)
1600.	60.974	61.169	61.347	61.506	61.646	61.767	61.867	61.945	62.002
1645.	61.322	61.517	61.694	61.852	61.990	62.108	62.205	62.280	62.332
1650.	61.361	61.556	61.733	61.891	62.028	62.146	62.242	62.317	62.369
1665.	(61.478)	(61.673)	61.849	62.006	62.144	62.260	62.356	62.429	62.479
1665.	(61.478)	(61.673)	61.849	62.006	62.144	62.260	62.356	62.429	62.479
1697.15	(61.729)	(61.924)	(62.099)	(62.255)	(62.391)	(62.506)	(62.599)	(62.670)	(62.717)
1700.	(61.751)	(61.946)	(62.122)	(62.278)	(62.413)	(62.528)	(62.621)	(62.691)	(62.739)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.05. Molar entropy, S° [J/mol K)], of wustite, $Fe_{1-y}O$ for y = 0 to y = 0.16 between 200 and 1700 K at one bar total pressure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the molar entropy for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
200.	(45.385)	(44.239)	(43.074)	(41.889)	(40.685)	(39.460)	(38.214)	(36.945)	(35.654)
250.	(55.277)	(54.186)	(53.076)	(51.945)	(50.794)	(49.622)	(48.428)	(47.211)	(45.971)
273.15	(59.342)	(58.271)	(57.181)	(56.071)	(54.941)	(53.788)	(52.614)	(51.417)	(50.197)
298.15	(63.459)	(62.409)	(61.338)	(60.248)	(59.136)	(58.003)	(56.848)	(55.669)	(54.467)
300.	(63.754)	(62.704)	(61.635)	(60.546)	(59.436)	(58.304)	(57.150)	(55.973)	(54.771)
350.	(71.211)	(70.196)	(69.161)	(68.104)	(67.027)	(65.927)	(64.804)	(63.658)	(62.487)
400.	(77.837)	(76.850)	(75.843)	(74.815)	(73.764)	(72.691)	(71.595)	(70.475)	(69.330)
450.	(83.781)	(82.820)	(81.837)	(80.834)	(79.807)	(78.758)	(77.685)	(76.587)	(75.464)
500.	(89.164)	(88.226)	(87.266)	(86.285)	(85.280)	(84.252)	(83.200)	(82.122)	(81.019)
550.	(94.081)	(93.164)	(92.225)	(91.264)	(90.279)	(89.271)	(88.237)	(87.178)	(86.093)
600.	(98.605)	(97.708)	(96.789)	(95.847)	(94.880)	(93.890)	(92.874)	(91.832)	(90.764)
650.	(102.796)	(101.918)	(101.017)	(100.092)	(99.144)	(98.170)	(97.171)	(96.145)	(95.091)
700.	(106.701)	(105.841)	(104.957)	(104.050)	(103.117)	(102.159)	(101.175)	(100.164)	(99.125)
750.	(110.359)	(109.515)	(108.648)	(107.756)	(106.840)	(105.897)	(104.927)	(103.930)	(102.905)
800.	(113.800)	(112.973)	(112.121)	(111.245)	(110.343)	(109.414)	(108.459)	(107.475)	(106.462)
825.	(115.448)	(114.628)	(113.784)	(112.915)	(112.021)	(111.099)	(110.150)	(109.173)	(108.166)
839.15	(116.361)	(115.546)	(114.706)	(113.841)	(112.950)	(112.032)	(111.087)	(110.113)	(109.110)
850.	(117.051)	(116.239)	(115.403)	(114.541)	(113.653)	(112.738)	(111.796)	(110.825)	(109.824)
875.	(118.613)	(117.808)	(116.979)	(116.124)	(115.243)	(114.335)	(113.399)	(112.434)	111.439
900.	(120.134)	(119.337)	(118.515)	(117.667)	(116.793)	(115.891)	(114.961)	(114.002)	113.013
925.	(121.618)	(120.828)	(120.013)	(119.172)	(118.304)	(117.409)	(116.485)	115.532	114.548
950.	(123.067)	(122.284)	(121.475)	(120.641)	(119.780)	(118.890)	(117.973)	117.025	116.047
1000.	(125.864)	(125.095)	(124.301)	(123.479)	(122.630)	(121.753)	120.847	119.910	118.943
1050.	(128.541)	(127.786)	(127.004)	(126.195)	(125.358)	(124.492)	123.597	122.671	121.714
1100.	(131.108)	(130.366)	(129.596)	(128.799)	(127.974)	(127.120)	126.235	125.319	124.371
1150.	(133.575)	(132.845)	(132.088)	(131.303)	(130.489)	129.646	128.771	127.865	126.927
1184.	(135.201)	(134.479)	(133.730)	(132.953)	(132.146)	131.310	130.442	129.542	128.610
1184.	(135.201)	(134.479)	(133.730)	(132.953)	(132.146)	131.310	130.442	129.542	128.610
1200.	(135.952)	(135.234)	(134.489)	(133.715)	(132.912)	132.079	131.214	130.318	129.388
1250.	(138.245)	(137.539)	(136.805)	(136.042)	(135.250)	134.426	133.572	132.684	131.763
1300.	(140.461)	(139.766)	(139.044)	(138.292)	(137.510)	136.696	135.851	134.972	134.059
1350.	(142.606)	(141.923)	(141.212)	(140.470)	(139.698)	138.894	138.057	137.187	136.282
1400.	(144.687)	(144.015)	(143.313)	(142.582)	(141.820)	141.025	140.197	139.335	138.438
1450.	(146.706)	(146.045)	(145.354)	(144.633)	(143.880)	143.094	142.275	141.421	140.531
1500.	(148.670)	(148.019)	(147.338)	(146.626)	(145.883)	145.106	144.295	143.448	142.566
1550.	(150.581)	(149.940)	(149.269)	(148.567)	(147.832)	147.064	146.261	145.422	144.546
1600.	(152.442)	(151.812)	(151.151)	(150.458)	(149.732)	148.971	148.176	147.345	146.476
1645.	(154.079)	(153.457)	(152.805)	(152.120)	(151.401)	150.648	149.860	149.035	148.172
1650.	(154.258)	(153.638)	(152.986)	(152.302)	(151.585)	(150.832)	(150.045)	149.220	148.358
1665.	(154.795)	(154.177)	(153.528)	(152.847)	(152.132)	(151.382)	(150.597)	(149.774)	(148.914)
1665.	(154.795)	(154.177)	(153.528)	(152.847)	(152.132)	(151.382)	(150.597)	(149.774)	(148.914)
1697.15	(155.931)	(155.320)	(154.677)	(154.001)	(153.292)	(152.547)	(151.766)	(150.948)	(150.092)
1700.	(156.031)	(155.421)	(154.778)	(154.103)	(153.394)	(152.649)	(151.869)	(151.052)	(150.196)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

Table 9.05 Continued. Molar entropy, S° [J/mol K)], of wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
200.	(35.654)	(34.339)	(33.000)	(31.636)	(30.246)	(28.829)	(27.385)	(25.911)	(24.408)
250.	(45.971)	(44.707)	(43.419)	(42.104)	(40.763)	(39.395)	(37.998)	(36.572)	(35.115)
273.15	(50.197)	(48.952)	(47.682)	(46.386)	(45.063)	(43.713)	(42.333)	(40.924)	(39.484)
298.15	(54.467)	(53.240)	(51.987)	(50.709)	(49.403)	(48.069)	(46.707)	(45.314)	(43.890)
300.	(54.771)	(53.546)	(52.295)	(51.017)	(49.713)	(48.380)	(47.019)	(45.627)	(44.204)
350.	(62.487)	(61.291)	(60.070)	(58.821)	(57.545)	(56.240)	(54.905)	(53.540)	(52.143)
400.	(69.330)	(68.159)	(66.962)	(65.737)	(64.484)	(63.201)	(61.889)	(60.544)	(59.168)
450.	(75.464)	(74.315)	(73.139)	(71.934)	(70.701)	(69.438)	(68.144)	(66.818)	(65.458)
500.	(81.019)	(79.889)	(78.731)	(77.545)	(76.329)	(75.083)	(73.805)	(72.494)	(71.150)
550.	(86.093)	(84.980)	(83.840)	(82.670)	(81.470)	(80.238)	(78.975)	(77.678)	(76.346)
600.	(90.764)	(89.667)	(88.541)	(87.386)	(86.200)	(84.983)	(83.732)	(82.447)	(81.127)
650.	(95.091)	(94.009)	(92.898)	(91.757)	(90.584)	(89.379)	(88.140)	(86.867)	(85.557)
700.	(99.125)	(98.057)	(96.959)	(95.831)	(94.670)	(93.476)	(92.248)	(90.985)	(89.685)
750.	(102.905)	(101.850)	(100.764)	(99.647)	(98.498)	(97.315)	(96.097)	(94.843)	(93.552)
800.	(106.462)	(105.419)	(104.346)	(103.240)	(102.101)	(100.928)	(99.719)	(98.473)	(97.190)
825.	(108.166)	(107.129)	(106.061)	(104.960)	(103.826)	(102.658)	(101.454)	(100.212)	(98.932)
839.15	(109.110)	(108.076)	(107.011)	(105.914)	(104.782)	(103.616)	(102.415)	(101.175)	(99.898)
850.	(109.824)	(108.793)	(107.730)	(106.635)	(105.506)	(104.342)	(103.141)	(101.904)	(100.628)
875.	111.439	(110.413)	(109.356)	(108.265)	(107.141)	(105.981)	(104.785)	(103.551)	(102.279)
900.	113.013	(111.992)	(110.940)	(109.855)	(108.735)	(107.579)	(106.387)	(105.157)	(103.888)
925.	114.548	113.533	(112.486)	(111.405)	(110.290)	(109.138)	(107.950)	(106.723)	(105.457)
950.	116.047	115.037	(113.995)	(112.918)	(111.807)	(110.660)	(109.475)	(108.252)	(106.989)
1000.	118.943	117.943	(116.910)	(115.842)	(114.739)	(113.600)	(112.422)	(111.205)	(109.947)
1050.	121.714	120.723	119.699	(118.640)	(117.545)	(116.413)	(115.241)	(114.030)	(112.778)
1100.	124.371	123.390	122.375	(121.324)	(120.236)	(119.110)	(117.945)	(116.739)	(115.491)
1150.	126.927	125.954	124.947	123.903	(122.822)	(121.703)	(120.544)	(119.343)	(118.100)
1184.	128.610	127.643	126.641	125.603	(124.526)	(123.411)	(122.255)	(121.058)	(119.817)
1184.	128.610	127.643	126.641	125.603	(124.526)	(123.411)	(122.255)	(121.058)	(119.817)
1200.	129.388	128.424	127.424	126.388	(125.314)	(124.200)	(123.046)	(121.850)	(120.611)
1250.	131.763	130.807	129.815	128.785	127.718	(126.610)	(125.461)	(124.269)	(123.034)
1300.	134.059	133.111	132.126	131.103	130.041	(128.939)	(127.795)	(126.607)	(125.375)
1350.	136.282	135.341	134.363	133.347	132.291	131.193	(130.054)	(128.870)	(127.641)
1400.	138.438	137.504	136.533	135.522	134.471	133.379	(132.243)	(131.063)	(129.837)
1450.	140.531	139.604	138.639	137.634	136.589	135.501	(134.369)	(133.192)	(131.968)
1500.	142.566	141.645	140.686	139.687	138.647	137.563	136.435	(135.261)	(134.040)
1550.	144.546	143.632	142.679	141.685	140.649	139.570	138.445	(137.274)	(136.055)
1600.	146.476	145.568	144.621	143.632	142.601	141.525	140.404	139.235	138.017
1645.	148.172	147.270	146.327	145.343	144.315	143.243	142.124	140.958	139.742
1650.	148.358	147.456	146.514	145.531	144.503	143.431	142.313	141.147	139.931
1665.	(148.914)	(148.014)	147.074	146.091	145.065	143.994	142.877	141.711	140.496
1665.	(148.914)	(148.014)	147.074	146.091	145.065	143.994	142.877	141.711	140.496
1697.15	(150.092)	(149.196)	(148.259)	(147.279)	(146.256)	(145.187)	(144.072)	(142.908)	(141.693)
1700.	(150.196)	(149.300)	(148.363)	(147.384)	(146.361)	(145.292)	(144.177)	(143.013)	(141.798)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.06. Molar heat content (or incremental enthalpy), H°(T)-H°(298) (J/mol), of wustite, $Fe_{1-y}O$ for y = 0 to y = 0.16 between 200 and 1700 K at one bar total pressure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the molar heat content (or incremental enthalpy) for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
200.	(-4456.)	(-4479.)	(-4502.)	(-4525.)	(-4548.)	(-4570.)	(-4593.)	(-4615.)	(-4636.)
250.	(-2238.)	(-2249.)	(-2260.)	(-2271.)	(-2282.)	(-2293.)	(-2303.)	(-2314.)	(-2324.)
273.15	(-1176.)	(-1181.)	(-1187.)	(-1192.)	(-1198.)	(-1203.)	(-1209.)	(-1214.)	(-1219.)
298.15	(0.)	(0.)	(0.)	(0.)	(0.)	(0.)	(0.)	(0.)	(0.)
300.	(88.)	(88.)	(89.)	(89.)	(90.)	(90.)	(90.)	(91.)	(91.)
350.	(2508.)	(2519.)	(2531.)	(2542.)	(2553.)	(2563.)	(2574.)	(2584.)	(2595.)
400.	(4989.)	(5011.)	(5033.)	(5055.)	(5076.)	(5097.)	(5117.)	(5138.)	(5157.)
450.	(7513.)	(7546.)	(7578.)	(7610.)	(7642.)	(7673.)	(7703.)	(7733.)	(7762.)
500.	(10068.)	(10112.)	(10155.)	(10197.)	(10239.)	(10280.)	(10320.)	(10360.)	(10398.)
550.	(12647.)	(12702.)	(12757.)	(12810.)	(12862.)	(12913.)	(12963.)	(13012.)	(13060.)
600.	(15247.)	(15314.)	(15379.)	(15443.)	(15506.)	(15568.)	(15628.)	(15687.)	(15744.)
650.	(17866.)	(17944.)	(18021.)	(18096.)	(18169.)	(18242.)	(18312.)	(18381.)	(18448.)
700.	(20501.)	(20591.)	(20679.)	(20766.)	(20850.)	(20933.)	(21014.)	(21093.)	(21170.)
750.	(23151.)	(23254.)	(23354.)	(23452.)	(23548.)	(23642.)	(23733.)	(23822.)	(23909.)
800.	(25817.)	(25932.)	(26045.)	(26155.)	(26262.)	(26367.)	(26469.)	(26569.)	(26665.)
825.	(27156.)	(27277.)	(27396.)	(27512.)	(27625.)	(27736.)	(27843.)	(27948.)	(28049.)
839.15	(27916.)	(28041.)	(28163.)	(28282.)	(28399.)	(28512.)	(28623.)	(28730.)	(28835.)
850.	(28499.)	(28627.)	(28751.)	(28873.)	(28992.)	(29109.)	(29222.)	(29331.)	(29438.)
875.	(29845.)	(29979.)	(30111.)	(30239.)	(30364.)	(30485.)	(30604.)	(30719.)	30830.
900.	(31196.)	(31336.)	(31474.)	(31608.)	(31739.)	(31866.)	(31990.)	(32111.)	32227.
925.	(32550.)	(32697.)	(32841.)	(32981.)	(33118.)	(33251.)	(33381.)	33506.	33628.
950.	(33908.)	(34061.)	(34212.)	(34358.)	(34501.)	(34640.)	(34775.)	34906.	35033.
1000.	(36635.)	(36802.)	(36966.)	(37125.)	(37280.)	(37431.)	37577.	37719.	37856.
1050.	(39378.)	(39559.)	(39736.)	(39908.)	(40076.)	(40238.)	40396.	40548.	40696.
1100.	(42137.)	(42332.)	(42522.)	(42708.)	(42888.)	(43062.)	43231.	43395.	43552.
1150.	(44912.)	(45122.)	(45326.)	(45524.)	(45717.)	45903.	46084.	46258.	46426.
1184.	(46809.)	(47028.)	(47241.)	(47449.)	(47650.)	47845.	48034.	48216.	48391.
1184.	(46809.)	(47028.)	(47241.)	(47449.)	(47650.)	47845.	48034.	48216.	48391.
1200.	(47704.)	(47928.)	(48146.)	(48357.)	(48563.)	48762.	48954.	49140.	49318.
1250.	(50513.)	(50751.)	(50983.)	(51208.)	(51426.)	51638.	51842.	52038.	52227.
1300.	(53338.)	(53591.)	(53837.)	(54076.)	(54307.)	54531.	54747.	54955.	55155.
1350.	(56181.)	(56449.)	(56709.)	(56962.)	(57206.)	57443.	57671.	57890.	58100.
1400.	(59041.)	(59324.)	(59599.)	(59866.)	(60124.)	60373.	60613.	60843.	61064.
1450.	(61919.)	(62217.)	(62507.)	(62788.)	(63059.)	63321.	63573.	63815.	64046.
1500.	(64814.)	(65128.)	(65433.)	(65728.)	(66013.)	66288.	66552.	66805.	67047.
1550.	(67728.)	(68058.)	(68378.)	(68687.)	(68986.)	69274.	69550.	69815.	70067.
1600.	(70660.)	(71006.)	(71341.)	(71665.)	(71977.)	72278.	72567.	72843.	73106.
1645.	(73315.)	(73675.)	(74024.)	(74361.)	(74686.)	74999.	75299.	75585.	75858.
1650.	(73611.)	(73973.)	(74323.)	(74662.)	(74988.)	(75302.)	(75603.)	75891.	76164.
1665.	(74500.)	(74867.)	(75222.)	(75565.)	(75895.)	(76213.)	(76518.)	(76809.)	(77086.)
1665.	(74500.)	(74867.)	(75222.)	(75565.)	(75895.)	(76213.)	(76518.)	(76809.)	(77086.)
1697.15	(76411.)	(76788.)	(77153.)	(77505.)	(77845.)	(78171.)	(78484.)	(78782.)	(79066.)
1700.	(76581.)	(76959.)	(77325.)	(77678.)	(78018.)	(78345.)	(78659.)	(78958.)	(79242.)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

Table 9.06 Continued. Molar heat content (or incremental enthalpy), H°(T)-H°(298) (J/mol), of wustite, $Fe_{1-y}O$.

Temperature (K)	Composition of Wustite as "y" (moles) 0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
200.	(-4636.)	(-4658.)	(-4679.)	(-4700.)	(-4721.)	(-4741.)	(-4761.)	(-4781.)	(-4800.)
250.	(-2324.)	(-2334.)	(-2344.)	(-2354.)	(-2363.)	(-2373.)	(-2382.)	(-2391.)	(-2400.)
273.15	(-1219.)	(-1224.)	(-1229.)	(-1234.)	(-1239.)	(-1244.)	(-1249.)	(-1253.)	(-1258.)
298.15	(0.)	(0.)	(0.)	(0.)	(0.)	(0.)	(0.)	(0.)	(0.)
300.	(91.)	(92.)	(92.)	(92.)	(93.)	(93.)	(93.)	(94.)	(94.)
350.	(2595.)	(2605.)	(2615.)	(2624.)	(2634.)	(2643.)	(2652.)	(2661.)	(2670.)
400.	(5157.)	(5177.)	(5196.)	(5214.)	(5233.)	(5250.)	(5268.)	(5284.)	(5301.)
450.	(7762.)	(7791.)	(7818.)	(7846.)	(7872.)	(7898.)	(7923.)	(7948.)	(7971.)
500.	(10398.)	(10436.)	(10473.)	(10509.)	(10544.)	(10577.)	(10610.)	(10642.)	(10673.)
550.	(13060.)	(13107.)	(13153.)	(13197.)	(13240.)	(13282.)	(13322.)	(13361.)	(13399.)
600.	(15744.)	(15800.)	(15855.)	(15908.)	(15959.)	(16009.)	(16056.)	(16102.)	(16147.)
650.	(18448.)	(18513.)	(18576.)	(18638.)	(18697.)	(18755.)	(18810.)	(18863.)	(18914.)
700.	(21170.)	(21244.)	(21317.)	(21387.)	(21454.)	(21519.)	(21582.)	(21642.)	(21699.)
750.	(23909.)	(23993.)	(24074.)	(24153.)	(24229.)	(24301.)	(24371.)	(24438.)	(24501.)
800.	(26665.)	(26758.)	(26849.)	(26936.)	(27020.)	(27100.)	(27177.)	(27251.)	(27320.)
825.	(28049.)	(28147.)	(28242.)	(28334.)	(28422.)	(28506.)	(28587.)	(28663.)	(28736.)
839.15	(28835.)	(28936.)	(29033.)	(29127.)	(29217.)	(29304.)	(29386.)	(29465.)	(29539.)
850.	(29438.)	(29541.)	(29640.)	(29736.)	(29828.)	(29916.)	(30000.)	(30080.)	(30156.)
875.	30830.	(30938.)	(31042.)	(31142.)	(31238.)	(31330.)	(31418.)	(31501.)	(31579.)
900.	32227.	(32340.)	(32448.)	(32553.)	(32653.)	(32749.)	(32840.)	(32926.)	(33007.)
925.	33628.	33745.	(33859.)	(33967.)	(34072.)	(34171.)	(34265.)	(34355.)	(34439.)
950.	35033.	35155.	(35273.)	(35386.)	(35494.)	(35598.)	(35695.)	(35788.)	(35875.)
1000.	37856.	37988.	(38115.)	(38236.)	(38353.)	(38463.)	(38568.)	(38667.)	(38759.)
1050.	40696.	40837.	40973.	(41104.)	(41228.)	(41346.)	(41457.)	(41562.)	(41660.)
1100.	43552.	43704.	43849.	(43988.)	(44120.)	(44245.)	(44363.)	(44474.)	(44577.)
1150.	46426.	46588.	46742.	46890.	(47029.)	(47162.)	(47286.)	(47403.)	(47510.)
1184.	48391.	48559.	48720.	48873.	(49018.)	(49155.)	(49284.)	(49404.)	(49515.)
1184.	48391.	48559.	48720.	48873.	(49018.)	(49155.)	(49284.)	(49404.)	(49515.)
1200.	49318.	49489.	49653.	49809.	(49956.)	(50096.)	(50226.)	(50348.)	(50461.)
1250.	52227.	52408.	52581.	52745.	52901.	(53047.)	(53184.)	(53311.)	(53428.)
1300.	55155.	55345.	55527.	55700.	55863.	(56016.)	(56159.)	(56292.)	(56413.)
1350.	58100.	58301.	58492.	58673.	58843.	59003.	(59152.)	(59289.)	(59415.)
1400.	61064.	61274.	61474.	61664.	61842.	62008.	(62163.)	(62305.)	(62434.)
1450.	64046.	64266.	64476.	64673.	64858.	65031.	(65192.)	(65338.)	(65471.)
1500.	67047.	67277.	67495.	67701.	67894.	68073.	68239.	(68390.)	(68526.)
1550.	70067.	70307.	70534.	70748.	70948.	71133.	71304.	(71460.)	(71599.)
1600.	73106.	73356.	73592.	73814.	74021.	74212.	74388.	74548.	74690.
1645.	75858.	76116.	76360.	76589.	76802.	76999.	77180.	77343.	77488.
1650.	76164.	76424.	76669.	76899.	77112.	77310.	77491.	77654.	77799.
1665.	(77086.)	(77348.)	77596.	77828.	78044.	78243.	78425.	78590.	78736.
1665.	(77086.)	(77348.)	77596.	77828.	78044.	78243.	78425.	78590.	78736.
1697.15	(79066.)	(79335.)	(79588.)	(79825.)	(80046.)	(80249.)	(80434.)	(80601.)	(80748.)
1700.	(79242.)	(79512.)	(79765.)	(80003.)	(80221.)	(80427.)	(80612.)	(80779.)	(80927.)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.07. The Gibbs energy function, -[G°(T)-H°(298)]/T [J/(mol K)], of wustite, $Fe_{1-y}O$ for y = 0 to y = 0.16 between 200 and 1700 K at one bar total pressure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the Gibbs energy function for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
200.	(67.664)	(66.634)	(65.585)	(64.516)	(63.425)	(62.313)	(61.177)	(60.019)	(58.836)
250.	(64.230)	(63.184)	(62.117)	(61.030)	(59.922)	(58.793)	(57.641)	(56.466)	(55.267)
273.15	(63.646)	(62.596)	(61.527)	(60.437)	(59.326)	(58.194)	(57.039)	(55.861)	(54.660)
298.15	(63.459)	(62.409)	(61.338)	(60.248)	(59.136)	(58.003)	(56.848)	(55.669)	(54.467)
300.	(63.460)	(62.410)	(61.339)	(60.249)	(59.137)	(58.004)	(56.848)	(55.670)	(54.468)
350.	(64.046)	(62.998)	(61.930)	(60.842)	(59.733)	(58.603)	(57.450)	(56.274)	(55.074)
400.	(65.363)	(64.321)	(63.260)	(62.177)	(61.074)	(59.949)	(58.801)	(57.631)	(56.436)
450.	(67.085)	(66.051)	(64.997)	(63.922)	(62.826)	(61.708)	(60.567)	(59.403)	(58.216)
500.	(69.028)	(68.002)	(66.956)	(65.890)	(64.802)	(63.692)	(62.559)	(61.403)	(60.223)
550.	(71.085)	(70.069)	(69.031)	(67.973)	(66.894)	(65.792)	(64.668)	(63.519)	(62.347)
600.	(73.193)	(72.185)	(71.157)	(70.108)	(69.037)	(67.944)	(66.828)	(65.688)	(64.523)
650.	(75.311)	(74.312)	(73.293)	(72.252)	(71.191)	(70.106)	(68.998)	(67.867)	(66.710)
700.	(77.415)	(76.426)	(75.416)	(74.385)	(73.331)	(72.254)	(71.155)	(70.031)	(68.883)
750.	(79.491)	(78.510)	(77.509)	(76.487)	(75.443)	(74.375)	(73.283)	(72.167)	(71.027)
800.	(81.528)	(80.558)	(79.565)	(78.552)	(77.515)	(76.455)	(75.373)	(74.264)	(73.131)
825.	(82.531)	(81.564)	(80.577)	(79.567)	(78.536)	(77.480)	(76.401)	(75.297)	(74.167)
839.	(83.094)	(82.131)	(81.145)	(80.138)	(79.108)	(78.055)	(76.978)	(75.876)	(74.748)
850.	(83.523)	(82.561)	(81.578)	(80.572)	(79.544)	(78.493)	(77.418)	(76.318)	(75.191)
875.	(84.504)	(83.546)	(82.567)	(81.566)	(80.542)	(79.495)	(78.423)	(77.327)	76.204
900.	(85.472)	(84.519)	(83.544)	(82.547)	(81.528)	(80.484)	(79.416)	(78.324)	77.205
925.	(86.429)	(85.480)	(84.510)	(83.517)	(82.501)	(81.462)	(80.398)	79.309	78.193
950.	(87.375)	(86.430)	(85.463)	(84.474)	(83.463)	(82.426)	(81.367)	80.281	79.170
1000.	(89.229)	(88.293)	(87.335)	(86.354)	(85.350)	(84.322)	83.270	82.191	81.087
1050.	(91.038)	(90.111)	(89.160)	(88.187)	(87.191)	(86.170)	85.125	84.054	82.956
1100.	(92.801)	(91.882)	(90.939)	(89.974)	(88.985)	(87.973)	86.934	85.869	84.778
1150.	(94.521)	(93.609)	(92.675)	(91.717)	(90.736)	89.730	88.698	87.640	86.556
1184.	(95.666)	(94.759)	(93.830)	(92.878)	(91.901)	90.900	89.873	88.819	87.739
1184.	(95.666)	(94.759)	(93.830)	(92.878)	(91.901)	90.900	89.873	88.819	87.739
1200.	(96.199)	(95.294)	(94.368)	(93.417)	(92.443)	91.444	90.419	89.368	88.290
1250.	(97.835)	(96.938)	(96.019)	(95.076)	(94.109)	93.116	92.099	91.053	89.981
1300.	(99.432)	(98.542)	(97.631)	(96.695)	(95.735)	94.749	93.738	92.699	91.632
1350.	(100.991)	(100.109)	(99.205)	(98.276)	(97.323)	96.344	95.338	94.306	93.245
1400.	(102.515)	(101.641)	(100.742)	(99.821)	(98.875)	97.902	96.902	95.876	94.821
1450.	(104.004)	(103.137)	(102.246)	(101.331)	(100.391)	99.424	98.432	97.411	96.361
1500.	(105.461)	(104.600)	(103.716)	(102.807)	(101.874)	100.914	99.927	98.911	97.868
1550.	(106.885)	(106.032)	(105.154)	(104.253)	(103.325)	102.371	101.390	100.380	99.341
1600.	(108.279)	(107.433)	(106.563)	(105.667)	(104.746)	103.797	102.822	101.818	100.785
1645.	(109.510)	(108.670)	(107.806)	(106.916)	(105.999)	105.056	104.086	103.087	102.058
1650.	(109.645)	(108.806)	(107.942)	(107.052)	(106.138)	(105.194)	(104.225)	103.226	102.198
1665.	(110.050)	(109.212)	(108.350)	(107.463)	(106.549)	(105.608)	(104.640)	(103.643)	(102.616)
1665.	(110.050)	(109.212)	(108.350)	(107.463)	(106.549)	(105.608)	(104.640)	(103.643)	(102.616)
1697.15	(110.908)	(110.075)	(109.217)	(108.333)	(107.424)	(106.487)	(105.521)	(104.528)	(103.504)
1700.	(110.984)	(110.151)	(109.293)	(108.410)	(107.501)	(106.564)	(105.599)	(104.606)	(103.583)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

Table 9.07 Continued. The Gibbs energy function, -[G°(T)-H°(298)]/T [J/(mol K)], of wustite, $Fe_{1-y}O$.

Temperature (K)	Composition of Wustite as "y" (moles) 0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
200.	(58.836)	(57.629)	(56.396)	(55.137)	(53.850)	(52.534)	(51.190)	(49.815)	(48.408)
250.	(55.267)	(54.043)	(52.794)	(51.519)	(50.216)	(48.886)	(47.526)	(46.136)	(44.715)
273.15	(54.660)	(53.434)	(52.182)	(50.904)	(49.600)	(48.267)	(46.905)	(45.512)	(44.089)
298.15	(54.467)	(53.240)	(51.987)	(50.709)	(49.403)	(48.069)	(46.707)	(45.314)	(43.890)
300.	(54.468)	(53.241)	(51.988)	(50.710)	(49.404)	(48.070)	(46.708)	(45.315)	(43.891)
350.	(55.074)	(53.849)	(52.599)	(51.323)	(50.020)	(48.688)	(47.327)	(45.937)	(44.515)
400.	(56.436)	(55.217)	(53.972)	(52.701)	(51.402)	(50.076)	(48.720)	(47.333)	(45.916)
450.	(58.216)	(57.003)	(55.764)	(54.499)	(53.207)	(51.886)	(50.536)	(49.156)	(47.744)
500.	(60.223)	(59.017)	(57.786)	(56.528)	(55.242)	(53.928)	(52.585)	(51.210)	(49.804)
550.	(62.347)	(61.149)	(59.926)	(58.675)	(57.396)	(56.089)	(54.752)	(53.384)	(51.984)
600.	(64.523)	(63.333)	(62.117)	(60.874)	(59.602)	(58.302)	(56.971)	(55.610)	(54.216)
650.	(66.710)	(65.528)	(64.319)	(63.083)	(61.819)	(60.525)	(59.202)	(57.847)	(56.459)
700.	(68.883)	(67.708)	(66.507)	(65.278)	(64.021)	(62.734)	(61.417)	(60.068)	(58.686)
750.	(71.027)	(69.860)	(68.665)	(67.444)	(66.193)	(64.913)	(63.602)	(62.259)	(60.883)
800.	(73.131)	(71.971)	(70.785)	(69.570)	(68.326)	(67.053)	(65.747)	(64.410)	(63.040)
825.	(74.167)	(73.011)	(71.828)	(70.616)	(69.375)	(68.105)	(66.803)	(65.469)	(64.101)
839.	(74.748)	(73.594)	(72.413)	(71.204)	(69.964)	(68.695)	(67.396)	(66.063)	(64.697)
850.	(75.191)	(74.039)	(72.859)	(71.651)	(70.414)	(69.147)	(67.847)	(66.516)	(65.151)
875.	76.204	(75.055)	(73.879)	(72.674)	(71.440)	(70.175)	(68.879)	(67.550)	(66.188)
900.	77.205	(76.059)	(74.886)	(73.685)	(72.454)	(71.192)	(69.899)	(68.573)	(67.213)
925.	78.193	77.051	(75.882)	(74.684)	(73.456)	(72.196)	(70.906)	(69.583)	(68.226)
950.	79.170	78.031	(76.865)	(75.669)	(74.445)	(73.189)	(71.901)	(70.580)	(69.226)
1000.	81.087	79.955	(78.795)	(77.606)	(76.386)	(75.137)	(73.854)	(72.538)	(71.188)
1050.	82.956	81.830	80.677	(79.494)	(78.280)	(77.036)	(75.758)	(74.447)	(73.102)
1100.	84.778	83.659	82.512	(81.335)	(80.127)	(78.887)	(77.615)	(76.308)	(74.967)
1150.	86.556	85.443	84.302	83.130	(81.927)	(80.693)	(79.426)	(78.123)	(76.787)
1184.	87.739	86.631	85.493	84.325	(83.126)	(81.895)	(80.630)	(79.332)	(77.997)
1184.	87.739	86.631	85.493	84.325	(83.126)	(81.895)	(80.630)	(79.332)	(77.997)
1200.	88.290	87.183	86.047	84.881	(83.684)	(82.454)	(81.191)	(79.893)	(78.560)
1250.	89.981	88.880	87.750	86.589	85.397	(84.172)	(82.914)	(81.620)	(80.291)
1300.	91.632	90.538	89.413	88.257	87.069	(85.850)	(84.596)	(83.306)	(81.981)
1350.	93.245	92.155	91.036	89.886	88.703	87.487	(86.238)	(84.952)	(83.630)
1400.	94.821	93.737	92.623	91.477	90.298	89.087	(87.841)	(86.559)	(85.241)
1450.	96.361	95.282	94.173	93.032	91.859	90.652	(89.409)	(88.131)	(86.815)
1500.	97.868	96.794	95.689	94.553	93.385	92.181	90.943	(89.668)	(88.356)
1550.	99.341	98.273	97.173	96.041	94.876	93.678	92.442	(91.171)	(89.862)
1600.	100.785	99.721	98.626	97.499	96.338	95.142	93.912	92.643	91.336
1645.	102.058	100.999	99.907	98.784	97.627	96.435	95.206	93.941	92.637
1650.	102.198	101.138	100.048	98.926	97.768	96.576	95.349	94.084	92.780
1665.	(102.616)	(101.559)	100.470	99.348	98.192	97.001	95.775	94.510	93.207
1665.	(102.616)	(101.559)	100.470	99.348	98.192	97.001	95.775	94.510	93.207
1697.15	(103.504)	(102.450)	(101.364)	(100.244)	(99.091)	(97.903)	(96.678)	(95.416)	(94.114)
1700.	(103.583)	(102.529)	(101.442)	(100.324)	(99.171)	(97.982)	(96.758)	(95.496)	(94.194)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.08. Entropy change for formation, $\Delta_f S^\circ$[J/(mol K)], of wustite, $Fe_{1-y}O$, for $y = 0$ to $y = 0.16$ moles at 298.15 K and from 800 to 1700 K at one bar total pressure. The data in parentheses are for a metastable wustite. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the entropy change for the formation for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
298.15	(-66.433)	(-67.210)	(-68.007)	(-68.825)	(-69.663)	(-70.523)	(-71.406)	(-72.311)	(-73.240)
800.	(-61.048)	(-61.307)	(-61.590)	(-61.897)	(-62.231)	(-62.590)	(-62.977)	(-63.392)	(-63.836)
825.	(-61.111)	(-61.349)	(-61.613)	(-61.901)	(-62.215)	(-62.556)	(-62.924)	(-63.321)	(-63.746)
839.15	(-61.160)	(-61.388)	(-61.640)	(-61.917)	(-62.221)	(-62.551)	(-62.909)	(-63.295)	(-63.711)
850.	(-61.205)	(-61.424)	(-61.668)	(-61.937)	(-62.233)	(-62.555)	(-62.904)	(-63.283)	(-63.691)
875.	(-61.334)	(-61.534)	(-61.759)	(-62.009)	(-62.285)	(-62.589)	(-62.920)	(-63.281)	-63.671
900.	(-61.502)	(-61.682)	(-61.888)	(-62.119)	(-62.376)	(-62.661)	(-62.975)	(-63.317)	-63.689
925.	(-61.712)	(-61.873)	(-62.059)	(-62.271)	(-62.510)	(-62.776)	(-63.071)	-63.396	-63.750
950.	(-61.971)	(-62.113)	(-62.280)	(-62.473)	(-62.693)	(-62.941)	(-63.217)	-63.523	-63.860
1000.	(-62.695)	(-62.797)	(-62.924)	(-63.077)	(-63.259)	(-63.468)	-63.707	-63.976	-64.275
1050.	(-63.888)	(-63.946)	(-64.030)	(-64.141)	(-64.280)	(-64.447)	-64.645	-64.873	-65.133
1100.	(-64.460)	(-64.482)	(-64.530)	(-64.606)	(-64.710)	(-64.843)	-65.007	-65.201	-65.428
1150.	(-64.722)	(-64.711)	(-64.728)	(-64.773)	(-64.846)	-64.949	-65.083	-65.248	-65.447
1184.	(-64.823)	(-64.792)	(-64.789)	(-64.813)	(-64.867)	-64.951	-65.066	-65.213	-65.393
1184.	(-65.583)	(-65.544)	(-65.533)	(-65.550)	(-65.597)	-65.673	-65.780	-65.920	-66.092
1200.	(-65.527)	(-65.480)	(-65.460)	(-65.469)	(-65.508)	-65.576	-65.676	-65.808	-65.973
1250.	(-65.360)	(-65.287)	(-65.242)	(-65.227)	(-65.240)	-65.285	-65.361	-65.470	-65.612
1300.	(-65.207)	(-65.109)	(-65.039)	(-64.999)	(-64.989)	-65.010	-65.063	-65.149	-65.270
1350.	(-65.064)	(-64.942)	(-64.848)	(-64.784)	(-64.751)	-64.749	-64.780	-64.845	-64.945
1400.	(-64.932)	(-64.786)	(-64.669)	(-64.582)	(-64.526)	-64.502	-64.512	-64.555	-64.634
1450.	(-64.810)	(-64.640)	(-64.500)	(-64.390)	(-64.313)	-64.267	-64.256	-64.279	-64.338
1500.	(-64.696)	(-64.503)	(-64.340)	(-64.209)	(-64.110)	-64.043	-64.011	-64.014	-64.053
1550.	(-64.589)	(-64.374)	(-64.189)	(-64.037)	(-63.916)	-63.829	-63.777	-63.761	-63.781
1600.	(-64.489)	(-64.252)	(-64.046)	(-63.872)	(-63.731)	-63.624	-63.553	-63.517	-63.519
1645.	(-64.404)	(-64.148)	(-63.923)	(-63.731)	(-63.572)	-63.447	-63.358	-63.306	-63.291
1650.	(-64.395)	(-64.137)	(-63.910)	(-63.715)	(-63.554)	(-63.428)	(-63.337)	-63.283	-63.266
1665.	(-64.368)	(-64.103)	(-63.870)	(-63.670)	(-63.503)	(-63.370)	(-63.274)	(-63.214)	(-63.192)
1665.	(-64.871)	(-64.601)	(-64.363)	(-64.157)	(-63.985)	(-63.848)	(-63.746)	(-63.681)	(-63.655)
1697.15	(-64.876)	(-64.592)	(-64.341)	(-64.121)	(-63.936)	(-63.786)	(-63.671)	(-63.595)	(-63.556)
1700.	(-64.877)	(-64.592)	(-64.339)	(-64.118)	(-63.932)	(-63.780)	(-63.665)	(-63.587)	(-63.547)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

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Table 9.08 Continued. Entropy change for formation, $\Delta_f S^\circ$[J/(mol K)], of wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
298.15	(-73.240)	(-74.194)	(-75.173)	(-76.178)	(-77.211)	(-78.272)	(-79.361)	(-80.481)	(-81.632)
800.	(-63.836)	(-64.309)	(-64.814)	(-65.351)	(-65.921)	(-66.526)	(-67.166)	(-67.842)	(-68.557)
825.	(-63.746)	(-64.203)	(-64.690)	(-65.210)	(-65.763)	(-66.351)	(-66.974)	(-67.635)	(-68.334)
839.15	(-63.711)	(-64.157)	(-64.634)	(-65.145)	(-65.688)	(-66.267)	(-66.881)	(-67.533)	(-68.223)
850.	(-63.691)	(-64.130)	(-64.600)	(-65.102)	(-65.639)	(-66.210)	(-66.817)	(-67.462)	(-68.146)
875.	-63.671	(-64.092)	(-64.545)	(-65.031)	(-65.550)	(-66.105)	(-66.697)	(-67.326)	(-67.994)
900.	-63.689	(-64.093)	(-64.528)	(-64.997)	(-65.501)	(-66.039)	(-66.615)	(-67.228)	(-67.881)
925.	-63.750	-64.136	(-64.555)	(-65.007)	(-65.493)	(-66.015)	(-66.575)	(-67.173)	(-67.810)
950.	-63.860	-64.228	(-64.629)	(-65.064)	(-65.534)	(-66.040)	(-66.583)	(-67.165)	(-67.787)
1000.	-64.275	-64.608	(-64.973)	(-65.373)	(-65.808)	(-66.280)	(-66.790)	(-67.339)	(-67.929)
1050.	-65.133	-65.425	-65.751	(-66.112)	(-66.510)	(-66.944)	(-67.418)	(-67.931)	(-68.486)
1100.	-65.428	-65.688	-65.983	(-66.313)	(-66.680)	(-67.084)	(-67.528)	(-68.013)	(-68.540)
1150.	-65.447	-65.679	-65.946	-66.249	(-66.589)	(-66.968)	(-67.387)	(-67.847)	(-68.350)
1184.	-65.393	-65.607	-65.857	-66.143	(-66.466)	(-66.829)	(-67.232)	(-67.677)	(-68.165)
1184.	-66.092	-66.299	-66.541	-66.819	(-67.135)	(-67.490)	(-67.886)	(-68.323)	(-68.803)
1200.	-65.973	-66.172	-66.407	-66.678	(-66.988)	(-67.336)	(-67.726)	(-68.157)	(-68.632)
1250.	-65.612	-65.790	-66.003	-66.254	-66.543	(-66.872)	(-67.242)	(-67.655)	(-68.112)
1300.	-65.270	-65.426	-65.619	-65.849	-66.119	(-66.429)	(-66.781)	(-67.176)	(-67.616)
1350.	-64.945	-65.080	-65.253	-65.464	-65.714	-66.006	(-66.340)	(-66.719)	(-67.143)
1400.	-64.634	-64.750	-64.903	-65.095	-65.327	-65.601	(-65.918)	(-66.280)	(-66.688)
1450.	-64.338	-64.434	-64.568	-64.741	-64.956	-65.213	(-65.514)	(-65.860)	(-66.253)
1500.	-64.053	-64.130	-64.246	-64.402	-64.600	-64.840	-65.124	(-65.455)	(-65.834)
1550.	-63.781	-63.839	-63.937	-64.076	-64.256	-64.481	-64.750	(-65.066)	(-65.430)
1600.	-63.519	-63.559	-63.640	-63.761	-63.926	-64.134	-64.389	-64.690	-65.041
1645.	-63.291	-63.316	-63.381	-63.488	-63.638	-63.833	-64.074	-64.363	-64.702
1650.	-63.266	-63.289	-63.353	-63.458	-63.607	-63.800	-64.040	-64.327	-64.665
1665.	(-63.192)	(-63.210)	-63.269	-63.369	-63.513	-63.702	-63.937	-64.221	-64.554
1665.	(-63.655)	(-63.668)	-63.721	-63.816	-63.955	-64.139	-64.369	-64.648	-64.976
1697.15	(-63.556)	(-63.557)	(-63.599)	(-63.684)	(-63.812)	(-63.986)	(-64.206)	(-64.476)	(-64.795)
1700.	(-63.547)	(-63.548)	(-63.589)	(-63.672)	(-63.800)	(-63.972)	(-64.192)	(-64.461)	(-64.780)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.09. Enthalpy change for formation, $\Delta_f H°$[J/(mol K)], of wustite, $Fe_{1-y}O$, for y = 0 to y = 0.16 moles at 298.15 K and from 800 to 1700 K at one bar total pressure. The data in parentheses are for a metastable wustite. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the enthalpy change for the formation for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature (K)	Composition of Wustite as "y" (moles) 0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
298.15	(-262133.)	(-262770.)	(-263409.)	(-264047.)	(-264687.)	(-265326.)	(-265966.)	(-266606.)	(-267247.)
800.	(-259751.)	(-260119.)	(-260489.)	(-260863.)	(-261239.)	(-261619.)	(-262002.)	(-262388.)	(-262777.)
825.	(-259801.)	(-260153.)	(-260508.)	(-260866.)	(-261227.)	(-261591.)	(-261959.)	(-262330.)	(-262704.)
839.15	(-259842.)	(-260185.)	(-260531.)	(-260880.)	(-261232.)	(-261587.)	(-261946.)	(-262309.)	(-262675.)
850.	(-259881.)	(-260216.)	(-260555.)	(-260897.)	(-261242.)	(-261590.)	(-261943.)	(-262298.)	(-262658.)
875.	(-259992.)	(-260311.)	(-260633.)	(-260958.)	(-261287.)	(-261620.)	(-261956.)	(-262297.)	-262641.
900.	(-260141.)	(-260442.)	(-260747.)	(-261056.)	(-261368.)	(-261684.)	(-262004.)	(-262329.)	-262657.
925.	(-260333.)	(-260616.)	(-260904.)	(-261195.)	(-261490.)	(-261789.)	(-262093.)	-262401.	-262713.
950.	(-260576.)	(-260842.)	(-261111.)	(-261384.)	(-261662.)	(-261943.)	(-262230.)	-262520.	-262816.
1000.	(-261283.)	(-261510.)	(-261740.)	(-261975.)	(-262215.)	(-262459.)	-262708.	-262963.	-263222.
1050.	(-262507.)	(-262689.)	(-262875.)	(-263067.)	(-263263.)	(-263465.)	-263672.	-263884.	-264103.
1100.	(-263120.)	(-263263.)	(-263411.)	(-263564.)	(-263723.)	(-263888.)	-264058.	-264235.	-264418.
1150.	(-263414.)	(-263521.)	(-263633.)	(-263751.)	(-263876.)	-264006.	-264144.	-264288.	-264438.
1184.	(-263532.)	(-263615.)	(-263704.)	(-263799.)	(-263900.)	-264009.	-264124.	-264246.	-264376.
1184.	(-264431.)	(-264505.)	(-264585.)	(-264671.)	(-264764.)	-264863.	-264970.	-265083.	-265203.
1200.	(-264364.)	(-264428.)	(-264498.)	(-264575.)	(-264658.)	-264748.	-264845.	-264949.	-265061.
1250.	(-264161.)	(-264193.)	(-264232.)	(-264277.)	(-264331.)	-264391.	-264459.	-264535.	-264620.
1300.	(-263965.)	(-263965.)	(-263972.)	(-263987.)	(-264010.)	-264040.	-264079.	-264127.	-264183.
1350.	(-263777.)	(-263744.)	(-263719.)	(-263703.)	(-263695.)	-263696.	-263705.	-263724.	-263752.
1400.	(-263595.)	(-263530.)	(-263473.)	(-263425.)	(-263386.)	-263356.	-263336.	-263326.	-263326.
1450.	(-263421.)	(-263322.)	(-263232.)	(-263152.)	(-263082.)	-263021.	-262971.	-262931.	-262903.
1500.	(-263252.)	(-263120.)	(-262997.)	(-262884.)	(-262782.)	-262691.	-262610.	-262541.	-262484.
1550.	(-263089.)	(-262923.)	(-262767.)	(-262621.)	(-262487.)	-262364.	-262253.	-262154.	-262068.
1600.	(-262932.)	(-262731.)	(-262541.)	(-262363.)	(-262196.)	-262042.	-261900.	-261771.	-261655.
1645.	(-262795.)	(-262562.)	(-262342.)	(-262133.)	(-261937.)	-261754.	-261584.	-261428.	-261286.
1650.	(-262780.)	(-262544.)	(-262320.)	(-262108.)	(-261909.)	(-261722.)	(-261549.)	-261390.	-261245.
1665.	(-262735.)	(-262488.)	(-262254.)	(-262032.)	(-261823.)	(-261627.)	(-261445.)	(-261277.)	(-261123.)
1665.	(-263571.)	(-263317.)	(-263074.)	(-262844.)	(-262626.)	(-262422.)	(-262231.)	(-262055.)	(-261893.)
1697.15	(-263581.)	(-263303.)	(-263037.)	(-262784.)	(-262544.)	(-262318.)	(-262106.)	(-261909.)	(-261726.)
1700.	(-263582.)	(-263302.)	(-263034.)	(-262779.)	(-262537.)	(-262309.)	(-262095.)	(-261896.)	(-261712.)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

Table 9.09 Continued. Enthalpy change for formation, $\Delta_f H°$[J/(mol K)], of wustite, $Fe_{1-y}O$.

Temperature (K)	Composition of Wustite as "y" (moles) 0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
298.15	(-267247.)	(-267889.)	(-268531.)	(-269173.)	(-269816.)	(-270459.)	(-271103.)	(-271748.)	(-272393.)
800.	(-262777.)	(-263170.)	(-263566.)	(-263966.)	(-264370.)	(-264777.)	(-265189.)	(-265605.)	(-266026.)
825.	(-262704.)	(-263083.)	(-263465.)	(-263851.)	(-264241.)	(-264635.)	(-265034.)	(-265437.)	(-265845.)
839.15	(-262675.)	(-263045.)	(-263419.)	(-263797.)	(-264179.)	(-264565.)	(-264956.)	(-265352.)	(-265753.)
850.	(-262658.)	(-263022.)	(-263389.)	(-263761.)	(-264137.)	(-264517.)	(-264903.)	(-265293.)	(-265687.)
875.	-262641.	(-262989.)	(-263342.)	(-263699.)	(-264061.)	(-264427.)	(-264799.)	(-265175.)	(-265557.)
900.	-262657.	(-262990.)	(-263328.)	(-263670.)	(-264017.)	(-264369.)	(-264726.)	(-265088.)	(-265456.)
925.	-262713.	-263030.	(-263352.)	(-263678.)	(-264010.)	(-264347.)	(-264690.)	(-265038.)	(-265392.)
950.	-262816.	-263116.	(-263422.)	(-263732.)	(-264048.)	(-264370.)	(-264697.)	(-265031.)	(-265370.)
1000.	-263222.	-263487.	(-263758.)	(-264034.)	(-264317.)	(-264605.)	(-264900.)	(-265202.)	(-265510.)
1050.	-264103.	-264327.	-264557.	(-264794.)	(-265038.)	(-265288.)	(-265545.)	(-265810.)	(-266082.)
1100.	-264418.	-264608.	-264804.	(-265008.)	(-265218.)	(-265436.)	(-265662.)	(-265896.)	(-266138.)
1150.	-264438.	-264596.	-264762.	-264935.	(-265116.)	(-265305.)	(-265502.)	(-265709.)	(-265924.)
1184.	-264376.	-264513.	-264658.	-264811.	(-264973.)	(-265143.)	(-265322.)	(-265511.)	(-265709.)
1184.	-265203.	-265332.	-265468.	-265612.	(-265764.)	(-265926.)	(-266096.)	(-266275.)	(-266464.)
1200.	-265061.	-265181.	-265308.	-265444.	(-265589.)	(-265743.)	(-265905.)	(-266078.)	(-266260.)
1250.	-264620.	-264712.	-264814.	-264924.	-265044.	(-265173.)	(-265313.)	(-265463.)	(-265623.)
1300.	-264183.	-264249.	-264324.	-264409.	-264504.	(-264609.)	(-264725.)	(-264852.)	(-264991.)
1350.	-263752.	-263790.	-263839.	-263898.	-263968.	-264049.	(-264141.)	(-264246.)	(-264363.)
1400.	-263326.	-263336.	-263358.	-263391.	-263435.	-263492.	(-263561.)	(-263643.)	(-263739.)
1450.	-262903.	-262886.	-262880.	-262887.	-262906.	-262939.	(-262984.)	(-263044.)	(-263118.)
1500.	-262484.	-262439.	-262406.	-262387.	-262381.	-262388.	-262411.	(-262448.)	(-262500.)
1550.	-262068.	-261995.	-261935.	-261889.	-261857.	-261841.	-261839.	(-261854.)	(-261885.)
1600.	-261655.	-261554.	-261466.	-261394.	-261337.	-261295.	-261270.	-261262.	-261272.
1645.	-261286.	-261159.	-261047.	-260950.	-260870.	-260806.	-260760.	-260731.	-260722.
1650.	-261245.	-261115.	-261000.	-260901.	-260818.	-260752.	-260703.	-260673.	-260661.
1665.	(-261123.)	(-260984.)	-260861.	-260754.	-260663.	-260589.	-260533.	-260496.	-260478.
1665.	(-261893.)	(-261745.)	-261614.	-261498.	-261399.	-261317.	-261253.	-261207.	-261180.
1697.15	(-261726.)	(-261560.)	(-261409.)	(-261275.)	(-261158.)	(-261060.)	(-260979.)	(-260918.)	(-260876.)
1700.	(-261712.)	(-261543.)	(-261391.)	(-261256.)	(-261137.)	(-261037.)	(-260955.)	(-260892.)	(-260849.)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.10. Gibbs energy change for formation, $\Delta_f G°$[J/(mol K)], of wustite, $Fe_{1-y}O$, for y = 0 to y = 0.16 moles at 298.15 K and from 800 to 1700 K at one bar total pressure. The data in parentheses are for a metastable wustite. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the Gibbs energy change for the formation for the formula, FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
298.15	(-242326.)	(-242732.)	(-243132.)	(-243527.)	(-243916.)	(-244300.)	(-244676.)	(-245047.)	(-245411.)
800.	(-210912.)	(-211073.)	(-211218.)	(-211345.)	(-211455.)	(-211547.)	(-211620.)	(-211674.)	(-211708.)
825.	(-209385.)	(-209540.)	(-209678.)	(-209798.)	(-209900.)	(-209983.)	(-210047.)	(-210090.)	(-210114.)
839.15	(-208520.)	(-208672.)	(-208806.)	(-208922.)	(-209019.)	(-209098.)	(-209156.)	(-209195.)	(-209212.)
850.	(-207856.)	(-208005.)	(-208137.)	(-208250.)	(-208344.)	(-208419.)	(-208474.)	(-208508.)	(-208521.)
875.	(-206325.)	(-206468.)	(-206594.)	(-206700.)	(-206788.)	(-206855.)	(-206901.)	(-206926.)	-206929.
900.	(-204789.)	(-204928.)	(-205048.)	(-205149.)	(-205229.)	(-205289.)	(-205327.)	(-205344.)	-205337.
925.	(-203249.)	(-203384.)	(-203499.)	(-203594.)	(-203668.)	(-203721.)	(-203752.)	-203760.	-203744.
950.	(-201703.)	(-201834.)	(-201945.)	(-202035.)	(-202104.)	(-202150.)	(-202173.)	-202173.	-202149.
1000.	(-198588.)	(-198713.)	(-198816.)	(-198898.)	(-198956.)	(-198991.)	-199002.	-198987.	-198947.
1050.	(-195425.)	(-195546.)	(-195644.)	(-195719.)	(-195769.)	(-195795.)	-195794.	-195768.	-195713.
1100.	(-192214.)	(-192333.)	(-192428.)	(-192498.)	(-192542.)	(-192560.)	-192551.	-192514.	-192447.
1150.	(-188984.)	(-189103.)	(-189196.)	(-189263.)	(-189303.)	-189315.	-189298.	-189252.	-189175.
1184.	(-186782.)	(-186901.)	(-186994.)	(-187060.)	(-187098.)	-187106.	-187086.	-187034.	-186950.
1184.	(-186782.)	(-186901.)	(-186994.)	(-187060.)	(-187098.)	-187106.	-187086.	-187034.	-186950.
1200.	(-185733.)	(-185853.)	(-185946.)	(-186012.)	(-186049.)	-186057.	-186034.	-185980.	-185894.
1250.	(-182461.)	(-182584.)	(-182678.)	(-182744.)	(-182780.)	-182785.	-182758.	-182698.	-182604.
1300.	(-179196.)	(-179324.)	(-179421.)	(-179489.)	(-179524.)	-179528.	-179498.	-179433.	-179332.
1350.	(-175940.)	(-176073.)	(-176174.)	(-176244.)	(-176281.)	-176284.	-176252.	-176183.	-176077.
1400.	(-172690.)	(-172829.)	(-172936.)	(-173010.)	(-173049.)	-173053.	-173019.	-172948.	-172838.
1450.	(-169446.)	(-169594.)	(-169707.)	(-169786.)	(-169828.)	-169833.	-169800.	-169727.	-169613.
1500.	(-166209.)	(-166365.)	(-166486.)	(-166571.)	(-166618.)	-166626.	-166594.	-166520.	-166404.
1550.	(-162977.)	(-163143.)	(-163273.)	(-163365.)	(-163417.)	-163429.	-163399.	-163326.	-163208.
1600.	(-159750.)	(-159928.)	(-160067.)	(-160167.)	(-160226.)	-160243.	-160216.	-160144.	-160025.
1645.	(-156850.)	(-157039.)	(-157188.)	(-157296.)	(-157362.)	-157384.	-157360.	-157290.	-157172.
1650.	(-156528.)	(-156718.)	(-156868.)	(-156977.)	(-157044.)	(-157066.)	(-157043.)	-156974.	-156856.
1665.	(-155562.)	(-155756.)	(-155910.)	(-156022.)	(-156091.)	(-156115.)	(-156094.)	(-156025.)	(-155907.)
1665.	(-155562.)	(-155756.)	(-155910.)	(-156022.)	(-156091.)	(-156115.)	(-156094.)	(-156025.)	(-155907.)
1697.15	(-153476.)	(-153679.)	(-153841.)	(-153960.)	(-154035.)	(-154064.)	(-154046.)	(-153979.)	(-153862.)
1700.	(-153291.)	(-153495.)	(-153658.)	(-153777.)	(-153852.)	(-153882.)	(-153864.)	(-153798.)	(-153681.)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

Table 9.10 Continued. Gibbs Energy change for formation, $\Delta_f G°$[J/(mol K)], of wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
298.15	(-245411.)	(-245768.)	(-246118.)	(-246460.)	(-246795.)	(-247123.)	(-247442.)	(-247752.)	(-248055.)
800.	(-211708.)	(-211722.)	(-211714.)	(-211685.)	(-211633.)	(-211557.)	(-211457.)	(-211332.)	(-211181.)
825.	(-210114.)	(-210116.)	(-210096.)	(-210053.)	(-209987.)	(-209896.)	(-209780.)	(-209638.)	(-209469.)
839.15	(-209212.)	(-209207.)	(-209181.)	(-209131.)	(-209057.)	(-208958.)	(-208833.)	(-208682.)	(-208503.)
850.	(-208521.)	(-208512.)	(-208480.)	(-208424.)	(-208344.)	(-208239.)	(-208108.)	(-207950.)	(-207764.)
875.	-206929.	(-206909.)	(-206865.)	(-206797.)	(-206704.)	(-206585.)	(-206439.)	(-206265.)	(-206062.)
900.	-205337.	(-205307.)	(-205252.)	(-205172.)	(-205066.)	(-204933.)	(-204773.)	(-204583.)	(-204364.)
925.	-203744.	-203704.	(-203639.)	(-203547.)	(-203429.)	(-203283.)	(-203108.)	(-202903.)	(-202667.)
950.	-202149.	-202099.	(-202024.)	(-201921.)	(-201791.)	(-201632.)	(-201444.)	(-201224.)	(-200973.)
1000.	-198947.	-198880.	(-198785.)	(-198662.)	(-198509.)	(-198326.)	(-198110.)	(-197863.)	(-197581.)
1050.	-195713.	-195631.	-195519.	(-195376.)	(-195203.)	(-194996.)	(-194757.)	(-194482.)	(-194172.)
1100.	-192447.	-192351.	-192223.	(-192064.)	(-191871.)	(-191644.)	(-191381.)	(-191082.)	(-190745.)
1150.	-189175.	-189066.	-188924.	-188749.	(-188539.)	(-188292.)	(-188008.)	(-187685.)	(-187322.)
1184.	-186950.	-186834.	-186684.	-186498.	(-186277.)	(-186017.)	(-185719.)	(-185381.)	(-185001.)
1184.	-186950.	-186834.	-186684.	-186498.	(-186277.)	(-186017.)	(-185719.)	(-185381.)	(-185001.)
1200.	-185894.	-185774.	-185620.	-185430.	(-185204.)	(-184939.)	(-184634.)	(-184289.)	(-183902.)
1250.	-182604.	-182475.	-182310.	-182107.	-181865.	(-181584.)	(-181260.)	(-180894.)	(-180483.)
1300.	-179332.	-179195.	-179019.	-178805.	-178549.	(-178251.)	(-177910.)	(-177523.)	(-177090.)
1350.	-176077.	-175932.	-175748.	-175522.	-175253.	-174940.	(-174582.)	(-174176.)	(-173721.)
1400.	-172838.	-172687.	-172494.	-172258.	-171977.	-171650.	(-171275.)	(-170851.)	(-170375.)
1450.	-169613.	-169457.	-169257.	-169012.	-168720.	-168380.	(-167990.)	(-167548.)	(-167052.)
1500.	-166404.	-166243.	-166037.	-165784.	-165481.	-165129.	-164724.	(-164265.)	(-163750.)
1550.	-163208.	-163044.	-162832.	-162572.	-162260.	-161896.	-161477.	(-161002.)	(-160468.)
1600.	-160025.	-159859.	-159643.	-159376.	-159055.	-158680.	-158249.	-157758.	-157207.
1645.	-157172.	-157004.	-156785.	-156513.	-156185.	-155801.	-155358.	-154854.	-154287.
1650.	-156856.	-156688.	-156468.	-156195.	-155867.	-155482.	-155038.	-154533.	-153964.
1665.	(-155907.)	(-155739.)	-155519.	-155244.	-154914.	-154526.	-154078.	-153569.	-152995.
1665.	(-155907.)	(-155739.)	-155519.	-155244.	-154914.	-154526.	-154078.	-153569.	-152995.
1697.15	(-153862.)	(-153694.)	(-153472.)	(-153195.)	(-152860.)	(-152466.)	(-152011.)	(-151493.)	(-150909.)
1700.	(-153681.)	(-153513.)	(-153291.)	(-153013.)	(-152678.)	(-152284.)	(-151828.)	(-151309.)	(-150724.)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.11. The function $\bar{S}(Fe)-\bar{S}^\circ(Fe)$, J/(mol K), in wustite, $Fe_{1-y}O$, for y = 0 to y = 0.16 between 800 and 1700 K at one bar total presure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the function for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
800.	(25.479)	(27.850)	(30.294)	(32.814)	(35.413)	(38.094)	(40.861)	(43.718)	(46.669)
825.	(23.088)	(25.480)	(27.946)	(30.488)	(33.111)	(35.816)	(38.609)	(41.491)	(44.469)
839.15	(21.777)	(24.182)	(26.660)	(29.215)	(31.851)	(34.570)	(37.377)	(40.274)	(43.266)
850.	(20.792)	(23.206)	(25.694)	(28.259)	(30.905)	(33.634)	(36.452)	(39.360)	(42.364)
875.	(18.583)	(21.018)	(23.528)	(26.116)	(28.785)	(31.539)	(34.381)	(37.316)	40.346
900.	(16.453)	(18.909)	(21.441)	(24.052)	(26.745)	(29.523)	(32.390)	(35.350)	38.407
925.	(14.395)	(16.872)	(19.426)	(22.059)	(24.776)	(27.578)	(30.470)	33.456	36.540
950.	(12.402)	(14.901)	(17.477)	(20.132)	(22.872)	(25.698)	(28.615)	31.627	34.738
1000.	(8.592)	(11.133)	(13.754)	(16.455)	(19.241)	(22.116)	25.083	28.146	31.310
1050.	(4.988)	(7.573)	(10.237)	(12.984)	(15.817)	(18.740)	21.757	24.872	28.089
1100.	(1.565)	(4.192)	(6.900)	(9.692)	(12.572)	(15.544)	18.611	21.777	25.047
1150.	(-1.701)	(0.969)	(3.721)	(6.559)	(9.486)	12.506	15.622	18.840	22.163
1184.	(-3.840)	(-1.141)	(1.641)	(4.510)	(7.469)	10.521	13.672	16.925	20.284
1184.	(-5.570)	(-2.871)	(-0.089)	(2.780)	(5.739)	8.791	11.942	15.195	18.554
1200.	(-6.403)	(-3.690)	(-0.894)	(1.989)	(4.963)	8.031	11.198	14.467	17.843
1250.	(-8.950)	(-6.195)	(-3.354)	(-0.426)	(2.595)	5.711	8.928	12.248	15.678
1300.	(-11.420)	(-8.621)	(-5.737)	(-2.763)	(0.305)	3.469	6.736	10.108	13.591
1350.	(-13.820)	(-10.979)	(-8.051)	(-5.031)	(-1.917)	1.296	4.613	8.036	11.572
1400.	(-16.159)	(-13.275)	(-10.303)	(-7.238)	(-4.077)	-0.815	2.551	6.026	9.616
1450.	(-18.442)	(-15.516)	(-12.500)	(-9.389)	(-6.181)	-2.871	0.545	4.072	7.714
1500.	(-20.676)	(-17.707)	(-14.646)	(-11.490)	(-8.235)	-4.877	-1.411	2.167	5.863
1550.	(-22.863)	(-19.851)	(-16.747)	(-13.545)	(-10.244)	-6.837	-3.321	0.309	4.058
1600.	(-25.008)	(-21.954)	(-18.805)	(-15.558)	(-12.210)	-8.755	-5.189	-1.508	2.294
1645.	(-26.906)	(-23.813)	(-20.624)	(-17.337)	(-13.946)	-10.448	-6.837	-3.109	0.741
1650.	(-27.115)	(-24.017)	(-20.825)	(-17.533)	(-14.137)	(-10.634)	(-7.018)	-3.285	0.570
1665.	(-27.740)	(-24.629)	(-21.423)	(-18.118)	(-14.708)	(-11.190)	(-7.560)	(-3.811)	(0.060)
1665.	(-28.890)	(-25.780)	(-22.574)	(-19.269)	(-15.859)	(-12.341)	(-8.711)	(-4.962)	(-1.891)
1697.15	(-30.290)	(-27.152)	(-23.918)	(-20.583)	(-17.143)	(-13.595)	(-9.932)	(-6.150)	(-2.245)
1700.	(-30.413)	(-27.272)	(-24.035)	(-20.698)	(-17.256)	(-13.704)	(-10.039)	(-6.254)	(-2.346)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

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Table 9.11 Continued. The function $\bar{S}(Fe)-\bar{S}^\circ(Fe)$, J/(mol K), in wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
800.	(46.669)	(49.718)	(52.869)	(56.127)	(59.496)	(62.982)	(66.590)	(70.327)	(74.198)
825.	(44.469)	(47.545)	(50.724)	(54.011)	(57.411)	(60.928)	(64.569)	(68.340)	(72.245)
839.15	(43.266)	(46.358)	(49.553)	(52.857)	(56.274)	(59.809)	(63.469)	(67.258)	(71.184)
850.	(42.364)	(45.468)	(48.676)	(51.992)	(55.422)	(58.971)	(62.645)	(66.448)	(70.389)
875.	40.346	(43.478)	(46.713)	(50.059)	(53.520)	(57.100)	(60.806)	(64.644)	(68.619)
900.	38.407	(41.566)	(44.830)	(48.205)	(51.696)	(55.308)	(59.047)	(62.918)	(66.928)
925.	36.540	39.726	(43.019)	(46.423)	(49.944)	(53.587)	(57.359)	(61.264)	(65.309)
950.	34.738	37.951	(41.272)	(44.706)	(48.258)	(51.932)	(55.736)	(59.675)	(63.755)
1000.	31.310	34.578	(37.956)	(41.449)	(45.061)	(48.799)	(52.668)	(56.674)	(60.823)
1050.	28.089	31.412	34.847	(38.398)	(42.071)	(45.872)	(49.806)	(53.879)	(58.099)
1100.	25.047	28.425	31.917	(35.527)	(39.261)	(43.124)	(47.123)	(51.264)	(55.553)
1150.	22.163	25.597	29.145	32.814	(36.609)	(40.535)	(44.599)	(48.807)	(53.166)
1184.	20.284	23.755	27.342	31.051	(34.886)	(38.855)	(42.963)	(47.218)	(51.624)
1184.	18.554	22.025	25.612	29.321	(33.157)	(37.125)	(41.234)	(45.488)	(49.894)
1200.	17.843	21.332	24.937	28.664	(32.520)	(36.509)	(40.638)	(44.913)	(49.342)
1250.	15.678	19.221	22.884	26.670	30.586	(34.638)	(38.832)	(43.175)	(47.673)
1300.	13.591	17.189	20.908	24.753	28.730	(32.844)	(37.104)	(41.514)	(46.083)
1350.	11.572	15.226	19.001	22.905	26.943	31.120	(35.444)	(39.922)	(44.561)
1400.	9.616	13.324	17.156	21.119	25.217	29.457	(33.847)	(38.392)	(43.100)
1450.	7.714	11.477	15.367	19.388	23.547	27.850	(32.304)	(36.917)	(41.695)
1500.	5.863	9.681	13.627	17.707	21.927	26.293	30.813	(35.492)	(40.340)
1550.	4.058	7.931	11.934	16.072	20.353	24.782	29.366	(34.114)	(39.031)
1600.	2.294	6.222	10.282	14.480	18.821	23.313	27.962	32.777	37.764
1645.	0.741	4.718	8.829	13.080	17.476	22.024	26.732	31.607	36.657
1650.	0.570	4.553	8.670	12.926	17.328	21.882	26.597	31.479	36.536
1665.	(0.060)	(4.059)	8.193	12.467	16.887	21.461	26.195	31.097	36.175
1665.	(-1.091)	(2.908)	7.042	11.316	15.736	20.310	25.044	29.946	35.024
1697.15	(-2.245)	(1.790)	(5.960)	(10.272)	(14.731)	(19.345)	(24.121)	(29.067)	(34.189)
1700.	(-2.346)	(1.692)	(5.866)	(10.181)	(14.643)	(19.261)	(24.041)	(28.990)	(34.117)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.12. The function $\overline{H}(Fe)-\overline{H}^{\circ}(Fe)$, J/(mol K), in wustite, $Fe_{1-y}O$, for y = 0 to y = 0.16 between 800 and 1700 K at one bar total presure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the function for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
800.	(37306.)	(37579.)	(37861.)	(38152.)	(38452.)	(38761.)	(39081.)	(39411.)	(39751.)
825.	(35363.)	(35654.)	(35954.)	(36263.)	(36582.)	(36911.)	(37251.)	(37601.)	(37963.)
839.15	(34273.)	(34574.)	(34884.)	(35204.)	(35534.)	(35874.)	(36226.)	(36588.)	(36963.)
850.	(33441.)	(33749.)	(34068.)	(34396.)	(34735.)	(35084.)	(35444.)	(35817.)	(36201.)
875.	(31536.)	(31863.)	(32200.)	(32548.)	(32907.)	(33277.)	(33659.)	(34053.)	34461.
900.	(29645.)	(29991.)	(30348.)	(30716.)	(31096.)	(31487.)	(31892.)	(32309.)	32740.
925.	(27767.)	(28133.)	(28510.)	(28898.)	(29299.)	(29713.)	(30140.)	30581.	31036.
950.	(25898.)	(26284.)	(26682.)	(27092.)	(27515.)	(27951.)	(28401.)	28866.	29347.
1000.	(22185.)	(22612.)	(23053.)	(23507.)	(23976.)	(24459.)	24958.	25473.	26005.
1050.	(18492.)	(18964.)	(19449.)	(19950.)	(20467.)	(21000.)	21550.	22118.	22704.
1100.	(14812.)	(15330.)	(15863.)	(16413.)	(16980.)	(17564.)	18168.	18792.	19435.
1150.	(11139.)	(11705.)	(12287.)	(12888.)	(13508.)	14147.	14807.	15488.	16192.
1184.	(8643.)	(9242.)	(9860.)	(10497.)	(11154.)	11831.	12531.	13253.	13999.
1184.	(6595.)	(7194.)	(7812.)	(8449.)	(9105.)	9783.	10483.	11205.	11951.
1200.	(5602.)	(6217.)	(6852.)	(7506.)	(8181.)	8877.	9595.	10337.	11103.
1250.	(2482.)	(3150.)	(3838.)	(4548.)	(5280.)	6036.	6815.	7620.	8451.
1300.	(-666.)	(56.)	(801.)	(1568.)	(2360.)	3177.	4021.	4891.	5790.
1350.	(-3847.)	(-3068.)	(-2265.)	(-1437.)	(-583.)	298.	1208.	2147.	3116.
1400.	(-7063.)	(-6225.)	(-5361.)	(-4471.)	(-3552.)	-2605.	-1627.	-617.	426.
1450.	(-10316.)	(-9418.)	(-8491.)	(-7536.)	(-6551.)	-5534.	-4485.	-3402.	-2284.
1500.	(-13610.)	(-12648.)	(-11657.)	(-10635.)	(-9580.)	-8493.	-7370.	-6211.	-5014.
1550.	(-16946.)	(-15919.)	(-14860.)	(-13769.)	(-12643.)	-11481.	-10283.	-9045.	-7767.
1600.	(-20324.)	(-19230.)	(-18102.)	(-16939.)	(-15740.)	-14502.	-13225.	-11906.	-10544.
1645.	(-23403.)	(-22246.)	(-21054.)	(-19824.)	(-18556.)	-17248.	-15898.	-14504.	-13064.
1650.	(-23747.)	(-22583.)	(-21384.)	(-20147.)	(-18871.)	(-17555.)	(-16197.)	-14794.	-13346.
1665.	(-24783.)	(-23598.)	(-22376.)	(-21117.)	(-19818.)	(-18477.)	(-17094.)	(-15666.)	(-14191.)
1665.	(-26699.)	(-25514.)	(-24293.)	(-23033.)	(-21734.)	(-20394.)	(-19011.)	(-17583.)	(-16108.)
1697.15	(-29052.)	(-27821.)	(-26551.)	(-25243.)	(-23893.)	(-22501.)	(-21064.)	(-19580.)	(-18047.)
1700.	(-29260.)	(-28025.)	(-26751.)	(-25438.)	(-24084.)	(-22687.)	(-21245.)	(-19756.)	(-18219.)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

Table 9.12 Continued. The function $\overline{H}(Fe)-\overline{H}^{\circ}(Fe)$, J/(mol K), in wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
800.	(39751.)	(40103.)	(40466.)	(40842.)	(41231.)	(41633.)	(42050.)	(42481.)	(42928.)
825.	(37963.)	(38337.)	(38724.)	(39124.)	(39537.)	(39965.)	(40408.)	(40867.)	(41342.)
839.15	(36963.)	(37350.)	(37750.)	(38164.)	(38591.)	(39034.)	(39492.)	(39967.)	(40458.)
850.	(36201.)	(36598.)	(37009.)	(37433.)	(37872.)	(38326.)	(38796.)	(39283.)	(39787.)
875.	34461.	(34882.)	(35317.)	(35766.)	(36231.)	(36713.)	(37211.)	(37727.)	(38261.)
900.	32740.	(33185.)	(33645.)	(34121.)	(34613.)	(35122.)	(35649.)	(36195.)	(36760.)
925.	31036.	31506.	(31992.)	(32495.)	(33015.)	(33552.)	(34109.)	(34685.)	(35283.)
950.	29347.	29843.	(30355.)	(30885.)	(31434.)	(32001.)	(32588.)	(33196.)	(33826.)
1000.	26005.	26555.	(27123.)	(27710.)	(28318.)	(28946.)	(29597.)	(30271.)	(30969.)
1050.	22704.	23310.	23937.	(24584.)	(25254.)	(25947.)	(26664.)	(27407.)	(28177.)
1100.	19435.	20100.	20788.	(21499.)	(22234.)	(22994.)	(23781.)	(24597.)	(25441.)
1150.	16192.	16919.	17670.	18447.	(19250.)	(20082.)	(20942.)	(21833.)	(22756.)
1184.	13999.	14769.	15566.	16389.	(17241.)	(18122.)	(19034.)	(19979.)	(20957.)
1184.	11951.	12721.	13518.	14341.	(15193.)	(16074.)	(16986.)	(17930.)	(18909.)
1200.	11103.	11895.	12713.	13559.	(14434.)	(15339.)	(16276.)	(17246.)	(18251.)
1250.	8451.	9310.	10198.	11116.	12065.	(13047.)	(14064.)	(15116.)	(16207.)
1300.	5790.	6719.	7679.	8672.	9699.	(10761.)	(11861.)	(12999.)	(14179.)
1350.	3116.	4118.	5153.	6224.	7331.	8477.	(9662.)	(10890.)	(12162.)
1400.	426.	1503.	2617.	3768.	4959.	6191.	(7466.)	(8786.)	(10154.)
1450.	-2284.	-1128.	67.	1302.	2579.	3900.	(5268.)	(6685.)	(8152.)
1500.	-5014.	-3777.	-2499.	-1177.	190.	1604.	3068.	(4584.)	(6154.)
1550.	-7767.	-6446.	-5081.	-3670.	-2211.	-701.	863.	(2481.)	(4158.)
1600.	-10544.	-9137.	-7682.	-6178.	-4623.	-3014.	-1349.	376.	2163.
1645.	-13064.	-11577.	-10040.	-8450.	-6806.	-5105.	-3345.	-1522.	367.
1650.	-13346.	-11849.	-10302.	-8703.	-7049.	-5338.	-3567.	-1733.	167.
1665.	(-14191.)	(-12667.)	-11092.	-9464.	-7780.	-6038.	-4234.	-2366.	-431.
1665.	(-16108.)	(-14584.)	-13009.	-11381.	-9697.	-7954.	-6151.	-4283.	-2348.
1697.15	(-18047.)	(-16464.)	(-14828.)	(-13136.)	(-11386.)	(-9576.)	(-7702.)	(-5761.)	(-3751.)
1700.	(-18219.)	(-16630.)	(-14988.)	(-13291.)	(-11535.)	(-9719.)	(-7838.)	(-5891.)	(-3874.)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.13. The function $\overline{G}(Fe)-\overline{G}^{\circ}(Fe)$, J/(mol K), in wustite, $Fe_{1-y}O$, for y = 0 to y = 0.16 between 800 and 1700 K at one bar total presure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the function for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
800.	(16922.)	(15299.)	(13626.)	(11901.)	(10122.)	(8286.)	(6392.)	(4436.)	(2416.)
825.	(16315.)	(14633.)	(12898.)	(11110.)	(9266.)	(7363.)	(5399.)	(3371.)	(1277.)
839.15	(15998.)	(14281.)	(12512.)	(10688.)	(8806.)	(6865.)	(4861.)	(2792.)	(656.)
850.	(15767.)	(14024.)	(12228.)	(10376.)	(8466.)	(6495.)	(4460.)	(2360.)	(191.)
875.	(15275.)	(13472.)	(11613.)	(9696.)	(7720.)	(5680.)	(3575.)	(1402.)	-842.
900.	(14837.)	(12973.)	(11051.)	(9069.)	(7026.)	(4917.)	(2741.)	(494.)	-1827.
925.	(14452.)	(12526.)	(10540.)	(8493.)	(6382.)	(4203.)	(1955.)	-366.	-2763.
950.	(14117.)	(12129.)	(10079.)	(7966.)	(5786.)	(3538.)	(1217.)	-1179.	-3654.
1000.	(13593.)	(11479.)	(9299.)	(7052.)	(4734.)	(2343.)	-125.	-2673.	-5304.
1050.	(13254.)	(11012.)	(8700.)	(6317.)	(3859.)	(1323.)	-1295.	-3998.	-6789.
1100.	(13091.)	(10718.)	(8273.)	(5751.)	(3150.)	(466.)	-2304.	-5163.	-8116.
1150.	(13095.)	(10590.)	(8008.)	(5345.)	(2599.)	-234.	-3159.	-6178.	-9296.
1184.	(13190.)	(10593.)	(7917.)	(5157.)	(2311.)	-626.	-3657.	-6786.	-10017.
1184.	(13190.)	(10593.)	(7917.)	(5157.)	(2311.)	-626.	-3657.	-6786.	-10017.
1200.	(13285.)	(10646.)	(7925.)	(5119.)	(2225.)	-760.	-3842.	-7023.	-10309.
1250.	(13670.)	(10893.)	(8031.)	(5080.)	(2037.)	-1104.	-4344.	-7690.	-11146.
1300.	(14179.)	(11264.)	(8259.)	(5160.)	(1965.)	-1333.	-4736.	-8249.	-11878.
1350.	(14810.)	(11754.)	(8604.)	(5355.)	(2005.)	-1452.	-5019.	-8702.	-12507.
1400.	(15560.)	(12361.)	(9063.)	(5662.)	(2155.)	-1463.	-5198.	-9054.	-13036.
1450.	(16425.)	(13081.)	(9633.)	(6078.)	(2412.)	-1371.	-5275.	-9306.	-13469.
1500.	(17404.)	(13911.)	(10312.)	(6600.)	(2772.)	-1177.	-5253.	-9462.	-13808.
1550.	(18492.)	(14851.)	(11097.)	(7227.)	(3235.)	-884.	-5135.	-9523.	-14056.
1600.	(19689.)	(15896.)	(11986.)	(7954.)	(3796.)	-494.	-4922.	-9493.	-14215.
1645.	(20857.)	(16926.)	(12873.)	(8695.)	(4385.)	-62.	-4651.	-9389.	-14283.
1650.	(20992.)	(17045.)	(12977.)	(8782.)	(4455.)	(-9.)	(-4617.)	-9373.	-14286.
1665.	(21404.)	(17410.)	(13294.)	(9049.)	(4671.)	(154.)	(-4507.)	(-9320.)	(-14291.)
1665.	(21403.)	(17410.)	(13293.)	(9049.)	(4671.)	(154.)	(-4508.)	(-9320.)	(-14291.)
1697.15	(22355.)	(18261.)	(14041.)	(9689.)	(5202.)	(571.)	(-4208.)	(-9142.)	(-14237.)
1700.	(22441.)	(18338.)	(14109.)	(9748.)	(5251.)	(610.)	(-4179.)	(-9124.)	(-14231.)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

Table 9.13 Continued. The function $\overline{G}(Fe)-\overline{G}^{\circ}(Fe)$, J/(mol K), in wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
800.	(2416.)	(328.)	(-1829.)	(-4059.)	(-6366.)	(-8752.)	(-11223.)	(-13781.)	(-16431.)
825.	(1277.)	(-887.)	(-3123.)	(-5435.)	(-7827.)	(-10301.)	(-12862.)	(-15514.)	(-18261.)
839.15	(656.)	(-1552.)	(-3833.)	(-6192.)	(-8631.)	(-11155.)	(-13768.)	(-16473.)	(-19276.)
850.	(191.)	(-2050.)	(-4366.)	(-6760.)	(-9237.)	(-11799.)	(-14452.)	(-17199.)	(-20044.)
875.	-842.	(-3161.)	(-5558.)	(-8036.)	(-10599.)	(-13250.)	(-15995.)	(-18837.)	(-21781.)
900.	-1827.	(-4224.)	(-6702.)	(-9264.)	(-11914.)	(-14655.)	(-17493.)	(-20431.)	(-23475.)
925.	-2763.	-5240.	(-7800.)	(-10447.)	(-13184.)	(-16016.)	(-18948.)	(-21984.)	(-25128.)
950.	-3654.	-6211.	(-8853.)	(-11586.)	(-14411.)	(-17335.)	(-20361.)	(-23495.)	(-26741.)
1000.	-5304.	-8023.	(-10833.)	(-13739.)	(-16743.)	(-19852.)	(-23071.)	(-26403.)	(-29855.)
1050.	-6789.	-9672.	-12653.	(-15734.)	(-18921.)	(-22218.)	(-25632.)	(-29166.)	(-32827.)
1100.	-8116.	-11168.	-14321.	(-17581.)	(-20954.)	(-24442.)	(-28054.)	(-31794.)	(-35668.)
1150.	-9296.	-12517.	-15847.	-19289.	(-22850.)	(-26533.)	(-30346.)	(-34295.)	(-38385.)
1184.	-10017.	-13356.	-16807.	-20375.	(-24065.)	(-27883.)	(-31835.)	(-35927.)	(-40166.)
1184.	-10017.	-13356.	-16807.	-20375.	(-24065.)	(-27883.)	(-31835.)	(-35927.)	(-40166.)
1200.	-10309.	-13703.	-17211.	-20839.	(-24590.)	(-28472.)	(-32490.)	(-36650.)	(-40960.)
1250.	-11146.	-14717.	-18407.	-22222.	-26168.	(-30250.)	(-34476.)	(-38852.)	(-43385.)
1300.	-11878.	-15627.	-19501.	-23507.	-27650.	(-31937.)	(-36374.)	(-40969.)	(-45729.)
1350.	-12507.	-16437.	-20498.	-24698.	-29042.	-33536.	(-38188.)	(-43005.)	(-47995.)
1400.	-13036.	-17150.	-21402.	-25799.	-30345.	-35050.	(-39920.)	(-44962.)	(-50186.)
1450.	-13469.	-17770.	-22215.	-26811.	-31564.	-36482.	(-41573.)	(-46845.)	(-52306.)
1500.	-13808.	-18299.	-22940.	-27738.	-32701.	-37836.	-43151.	(-48655.)	(-54356.)
1550.	-14056.	-18739.	-23579.	-28583.	-33758.	-39112.	-44655.	(-50395.)	(-56340.)
1600.	-14215.	-19092.	-24134.	-29346.	-34737.	-40315.	-46088.	-52067.	-58260.
1645.	-14283.	-19339.	-24564.	-29966.	-35554.	-41335.	-47319.	-53515.	-59934.
1650.	-14286.	-19362.	-24607.	-30031.	-35641.	-41444.	-47452.	-53673.	-60117.
1665.	(-14291.)	(-19426.)	-24734.	-30222.	-35897.	-41769.	-47848.	-54143.	-60663.
1665.	(-14291.)	(-19427.)	-24734.	-30222.	-35898.	-41770.	-47849.	-54143.	-60663.
1697.15	(-14237.)	(-19502.)	(-24943.)	(-30569.)	(-36387.)	(-42407.)	(-48639.)	(-55091.)	(-61776.)
1700.	(-14231.)	(-19507.)	(-24960.)	(-30598.)	(-36429.)	(-42462.)	(-48707.)	(-55174.)	(-61873.)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.14. Activity of the Fe component, log a(Fe), in wustite, $Fe_{1-y}O$, for y = 0 to y = 0.16 between 800 and 1700 K at one bar total pressure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature.

Temperature	Composition of Wustite: first line = "y", second line = "x" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
	0.0000	0.0101	0.0204	0.0309	0.0417	0.0526	0.0638	0.0753	0.0870
800.	(1.1049)	(0.9989)	(0.8897)	(0.7770)	(0.6609)	(0.5410)	(0.4173)	(0.2896)	(0.1577)
825.	(1.0330)	(0.9264)	(0.8166)	(0.7034)	(0.5866)	(0.4661)	(0.3418)	(0.2134)	(0.0808)
839.15	(0.9958)	(0.8890)	(0.7788)	(0.6653)	(0.5481)	(0.4273)	(0.3026)	(0.1738)	(0.0408)
850.	(0.9689)	(0.8618)	(0.7514)	(0.6376)	(0.5202)	(0.3991)	(0.2741)	(0.1450)	(0.0118)
875.	(0.9118)	(0.8042)	(0.6932)	(0.5788)	(0.4608)	(0.3391)	(0.2134)	(0.0837)	-0.0503
900.	(0.8611)	(0.7529)	(0.6414)	(0.5264)	(0.4077)	(0.2854)	(0.1591)	(0.0287)	-0.1060
925.	(0.8161)	(0.7073)	(0.5952)	(0.4796)	(0.3604)	(0.2374)	(0.1104)	-0.0207	-0.1560
950.	(0.7762)	(0.6669)	(0.5542)	(0.4380)	(0.3181)	(0.1945)	(0.0669)	-0.0649	-0.2009
1000.	(0.7100)	(0.5996)	(0.4857)	(0.3684)	(0.2473)	(0.1224)	-0.0065	-0.1396	-0.2771
1050.	(0.6593)	(0.5478)	(0.4328)	(0.3142)	(0.1920)	(0.0658)	-0.0644	-0.1989	-0.3377
1100.	(0.6216)	(0.5090)	(0.3928)	(0.2731)	(0.1496)	(0.0221)	-0.1094	-0.2452	-0.3854
1150.	(0.5948)	(0.4810)	(0.3637)	(0.2428)	(0.1180)	-0.0106	-0.1435	-0.2806	-0.4222
1184.	(0.5819)	(0.4673)	(0.3493)	(0.2275)	(0.1019)	-0.0276	-0.1613	-0.2994	-0.4419
1184.	(0.5819)	(0.4673)	(0.3493)	(0.2275)	(0.1019)	-0.0276	-0.1613	-0.2994	-0.4419
1200.	(0.5783)	(0.4634)	(0.3449)	(0.2228)	(0.0969)	-0.0331	-0.1672	-0.3057	-0.4487
1250.	(0.5712)	(0.4552)	(0.3356)	(0.2123)	(0.0851)	-0.0461	-0.1815	-0.3214	-0.4658
1300.	(0.5697)	(0.4526)	(0.3318)	(0.2073)	(0.0789)	-0.0535	-0.1903	-0.3314	-0.4772
1350.	(0.5730)	(0.4548)	(0.3329)	(0.2072)	(0.0776)	-0.0562	-0.1942	-0.3367	-0.4839
1400.	(0.5805)	(0.4612)	(0.3381)	(0.2113)	(0.0804)	-0.0546	-0.1939	-0.3378	-0.4864
1450.	(0.5917)	(0.4712)	(0.3470)	(0.2190)	(0.0869)	-0.0494	-0.1900	-0.3352	-0.4852
1500.	(0.6060)	(0.4844)	(0.3591)	(0.2298)	(0.0965)	-0.0410	-0.1829	-0.3295	-0.4808
1550.	(0.6232)	(0.5004)	(0.3740)	(0.2435)	(0.1090)	-0.0298	-0.1730	-0.3209	-0.4737
1600.	(0.6428)	(0.5189)	(0.3913)	(0.2597)	(0.1239)	-0.0161	-0.1607	-0.3099	-0.4640
1645.	(0.6623)	(0.5374)	(0.4088)	(0.2761)	(0.1392)	-0.0020	-0.1477	-0.2981	-0.4535
1650.	(0.6645)	(0.5396)	(0.4108)	(0.2780)	(0.1410)	(-0.0003)	(-0.1461)	-0.2967	-0.4522
1665.	(0.6715)	(0.5462)	(0.4170)	(0.2839)	(0.1465)	(0.0048)	(-0.1414)	(-0.2924)	(-0.4483)
1665.	(0.6715)	(0.5462)	(0.4170)	(0.2839)	(0.1465)	(0.0048)	(-0.1414)	(-0.2924)	(-0.4483)
1697.15	(0.6880)	(0.5620)	(0.4321)	(0.2982)	(0.1601)	(0.0176)	(-0.1295)	(-0.2814)	(-0.4382)
1700.	(0.6895)	(0.5635)	(0.4335)	(0.2995)	(0.1613)	(0.0187)	(-0.1284)	(-0.2803)	(-0.4373)

Table 9.14 Continued. Activity of the Fe component, log a(Fe), in wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite: first line = "y", second line = "x" (moles)								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
	0.0870	0.0999	0.1111	0.1236	0.1364	0.1494	0.1628	0.1765	0.1905
800.	(0.1577)	(0.0214)	(-0.1194)	(-0.2650)	(-0.4156)	(-0.5714)	(-0.7327)	(-0.8998)	(-1.0728)
825.	(0.0808)	(-0.0562)	(-0.1978)	(-0.3441)	(-0.4955)	(-0.6522)	(-0.8143)	(-0.9822)	(-1.1562)
839.15	(0.0408)	(-0.0966)	(-0.2386)	(-0.3854)	(-0.5372)	(-0.6943)	(-0.8570)	(-1.0254)	(-1.1998)
850.	(0.0118)	(-0.1260)	(-0.2683)	(-0.4154)	(-0.5676)	(-0.7251)	(-0.8881)	(-1.0569)	(-1.2317)
875.	-0.0503	(-0.1887)	(-0.3318)	(-0.4797)	(-0.6327)	(-0.7910)	(-0.9548)	(-1.1245)	(-1.3002)
900.	-0.1060	(-0.2452)	(-0.3890)	(-0.5377)	(-0.6914)	(-0.8505)	(-1.0152)	(-1.1858)	(-1.3624)
925.	-0.1560	-0.2959	(-0.4405)	(-0.5899)	(-0.7445)	(-0.9044)	(-1.0700)	(-1.2414)	(-1.4189)
950.	-0.2009	-0.3415	(-0.4868)	(-0.6370)	(-0.7924)	(-0.9531)	(-1.1195)	(-1.2918)	(-1.4703)
1000.	-0.2771	-0.4191	(-0.5659)	(-0.7176)	(-0.8746)	(-1.0369)	(-1.2050)	(-1.3791)	(-1.5594)
1050.	-0.3377	-0.4812	-0.6294	(-0.7827)	(-0.9412)	(-1.1053)	(-1.2751)	(-1.4509)	(-1.6330)
1100.	-0.3854	-0.5303	-0.6800	(-0.8349)	(-0.9950)	(-1.1606)	(-1.3321)	(-1.5097)	(-1.6937)
1150.	-0.4222	-0.5685	-0.7198	-0.8761	(-1.0378)	(-1.2051)	(-1.3783)	(-1.5577)	(-1.7435)
1184.	-0.4419	-0.5892	-0.7415	-0.8989	(-1.0616)	(-1.2301)	(-1.4044)	(-1.5850)	(-1.7720)
1184.	-0.4419	-0.5892	-0.7415	-0.8989	(-1.0616)	(-1.2301)	(-1.4044)	(-1.5850)	(-1.7720)
1200.	-0.4487	-0.5965	-0.7492	-0.9071	(-1.0704)	(-1.2393)	(-1.4142)	(-1.5953)	(-1.7829)
1250.	-0.4658	-0.6150	-0.7691	-0.9286	-1.0935	(-1.2640)	(-1.4406)	(-1.6235)	(-1.8129)
1300.	-0.4772	-0.6279	-0.7835	-0.9445	-1.1110	(-1.2832)	(-1.4615)	(-1.6461)	(-1.8374)
1350.	-0.4839	-0.6360	-0.7931	-0.9556	-1.1237	-1.2975	(-1.4775)	(-1.6639)	(-1.8570)
1400.	-0.4864	-0.6399	-0.7985	-0.9625	-1.1322	-1.3077	(-1.4894)	(-1.6775)	(-1.8724)
1450.	-0.4852	-0.6401	-0.8003	-0.9658	-1.1370	-1.3142	(-1.4976)	(-1.6875)	(-1.8842)
1500.	-0.4808	-0.6372	-0.7988	-0.9659	-1.1387	-1.3175	-1.5026	(-1.6943)	(-1.8928)
1550.	-0.4737	-0.6315	-0.7946	-0.9632	-1.1376	-1.3180	-1.5048	(-1.6983)	(-1.8986)
1600.	-0.4640	-0.6233	-0.7879	-0.9580	-1.1340	-1.3161	-1.5046	-1.6998	-1.9019
1645.	-0.4535	-0.6141	-0.7800	-0.9515	-1.1289	-1.3125	-1.5025	-1.6993	-1.9031
1650.	-0.4522	-0.6129	-0.7790	-0.9507	-1.1283	-1.3120	-1.5022	-1.6991	-1.9031
1665.	(-0.4483)	(-0.6094)	-0.7759	-0.9481	-1.1261	-1.3104	-1.5011	-1.6985	-1.9031
1665.	(-0.4483)	(-0.6094)	-0.7759	-0.9481	-1.1262	-1.3104	-1.5011	-1.6985	-1.9031
1697.15	(-0.4382)	(-0.6002)	(-0.7677)	(-0.9408)	(-1.1199)	(-1.3052)	(-1.4970)	(-1.6956)	(-1.9013)
1700.	(-0.4373)	(-0.5994)	(-0.7669)	(-0.9401)	(-1.1193)	(-1.3047)	(-1.4966)	(-1.6953)	(-1.9011)

Table 9.15. The function $\bar{S}(O_2)-\bar{S}^\circ(O_2)$, J/(mol K), in wustite, $Fe_{1-y}O$, for y = 0 to y = 0.16 between 800 and 1700 K at one bar total presure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature., To obtain the function for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature (K)	Composition of Wustite as "y" (moles)								
	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
800.	(-171.468)	(-176.186)	(-181.000)	(-185.913)	(-190.929)	(-196.050)	(-201.281)	(-206.623)	(-212.082)
825.	(-167.630)	(-172.390)	(-177.248)	(-182.205)	(-187.266)	(-192.434)	(-197.711)	(-203.102)	(-208.610)
839.15	(-165.499)	(-170.284)	(-175.166)	(-180.149)	(-185.235)	(-190.429)	(-195.733)	(-201.151)	(-206.687)
850.	(-163.886)	(-168.689)	(-173.589)	(-178.591)	(-183.697)	(-188.911)	(-194.236)	(-199.675)	(-205.232)
875.	(-160.230)	(-165.076)	(-170.020)	(-175.066)	(-180.218)	(-185.477)	(-190.849)	(-196.336)	-201.943
900.	(-156.659)	(-161.547)	(-166.535)	(-171.625)	(-176.822)	(-182.128)	(-187.546)	(-193.082)	-198.737
925.	(-153.167)	(-158.097)	(-163.128)	(-168.263)	(-173.505)	(-178.857)	(-184.323)	-189.906	-195.611
950.	(-149.749)	(-154.722)	(-159.797)	(-164.976)	(-170.263)	(-175.661)	(-181.174)	-186.806	-192.560
1000.	(-143.125)	(-148.183)	(-153.344)	(-158.612)	(-163.989)	(-169.480)	-175.087	-180.815	-186.668
1050.	(-136.757)	(-141.900)	(-147.148)	(-152.504)	(-157.972)	(-163.555)	-169.257	-175.081	-181.032
1100.	(-130.622)	(-135.850)	(-141.185)	(-146.630)	(-152.188)	(-157.863)	-163.659	-169.580	-175.629
1150.	(-124.699)	(-130.012)	(-135.434)	(-140.967)	(-146.616)	-152.384	-158.274	-164.291	-170.439
1184.	(-120.784)	(-126.155)	(-131.635)	(-137.229)	(-142.939)	-148.770	-154.724	-160.807	-167.021
1184.	(-120.784)	(-126.155)	(-131.635)	(-137.229)	(-142.939)	-148.770	-154.724	-160.807	-167.021
1200.	(-118.971)	(-124.369)	(-129.877)	(-135.499)	(-141.238)	-147.098	-153.083	-159.196	-165.443
1250.	(-113.420)	(-118.904)	(-124.499)	(-130.210)	(-136.039)	-141.991	-148.070	-154.280	-160.625
1300.	(-108.035)	(-113.603)	(-119.285)	(-125.084)	(-131.004)	-137.049	-143.222	-149.528	-155.971
1350.	(-102.801)	(-108.454)	(-114.223)	(-120.111)	(-126.121)	-132.258	-138.526	-144.928	-151.469
1400.	(-97.708)	(-103.446)	(-109.302)	(-115.278)	(-121.379)	-127.608	-133.970	-140.469	-147.109
1450.	(-92.745)	(-98.569)	(-104.512)	(-110.576)	(-116.768)	-123.089	-129.546	-136.141	-142.879
1500.	(-87.905)	(-93.814)	(-99.843)	(-105.997)	(-112.279)	-118.693	-125.243	-131.934	-138.771
1550.	(-83.180)	(-89.173)	(-95.289)	(-101.532)	(-107.904)	-114.410	-121.055	-127.842	-134.778
1600.	(-78.561)	(-84.639)	(-90.842)	(-97.173)	(-103.636)	-110.234	-116.973	-123.857	-130.891
1645.	(-74.489)	(-80.645)	(-86.926)	(-93.336)	(-99.880)	-106.562	-113.386	-120.357	-127.479
1650.	(-74.042)	(-80.206)	(-86.495)	(-92.915)	(-99.468)	(-106.159)	(-112.992)	-119.972	-127.104
1665.	(-72.705)	(-78.894)	(-85.210)	(-91.656)	(-98.236)	(-104.955)	(-111.816)	(-118.826)	(-125.987)
1665.	(-72.705)	(-78.894)	(-85.210)	(-91.656)	(-98.236)	(-104.955)	(-111.816)	(-118.826)	(-125.987)
1697.15	(-69.867)	(-76.111)	(-82.483)	(-88.986)	(-95.624)	(-102.402)	(-109.324)	(-116.395)	(-123.620)
1700.	(-69.617)	(-75.866)	(-82.243)	(-88.751)	(-95.394)	(-102.178)	(-109.105)	(-116.182)	(-123.412)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

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Table 9.15 Continued. The function $\bar{S}(O_2)-\bar{S}^\circ(O_2)$, J/(mol K), in wustite, $Fe_{1-y}O$.

Temperature (K)	Composition of Wustite as "y" (moles)								
	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
800.	(-212.082)	(-217.661)	(-223.364)	(-229.195)	(-235.158)	(-241.259)	(-247.501)	(-253.891)	(-260.432)
825.	(-208.610)	(-214.239)	(-219.993)	(-225.877)	(-231.894)	(-238.049)	(-244.348)	(-250.795)	(-257.395)
839.15	(-206.687)	(-212.344)	(-218.128)	(-224.041)	(-230.089)	(-236.275)	(-242.606)	(-249.086)	(-255.719)
850.	(-205.232)	(-210.911)	(-216.717)	(-222.653)	(-228.724)	(-234.934)	(-241.290)	(-247.794)	(-254.453)
875.	-201.943	(-207.672)	(-213.529)	(-219.518)	(-225.643)	(-231.908)	(-238.320)	(-244.882)	(-251.600)
900.	-198.737	(-204.517)	(-210.426)	(-216.467)	(-222.646)	(-228.966)	(-235.434)	(-242.054)	(-248.831)
925.	-195.611	-201.442	(-207.401)	(-213.495)	(-219.728)	(-226.103)	(-232.627)	(-239.304)	(-246.140)
950.	-192.560	-198.441	(-204.452)	(-210.599)	(-216.885)	(-223.315)	(-229.895)	(-236.630)	(-243.525)
1000.	-186.668	-192.649	(-198.763)	(-205.015)	(-211.408)	(-217.948)	(-224.641)	(-231.491)	(-238.504)
1050.	-181.032	-187.114	-193.331	(-199.688)	(-206.189)	(-212.839)	(-219.644)	(-226.610)	(-233.740)
1100.	-175.629	-181.812	-188.131	(-194.593)	(-201.202)	(-207.962)	(-214.880)	(-221.961)	(-229.210)
1150.	-170.439	-176.722	-183.144	-189.712	(-196.428)	(-203.298)	(-210.328)	(-217.524)	(-224.891)
1184.	-167.021	-173.373	-179.865	-186.504	(-193.293)	(-200.238)	(-207.345)	(-214.619)	(-222.066)
1184.	-167.021	-173.373	-179.865	-186.504	(-193.293)	(-200.238)	(-207.345)	(-214.619)	(-222.066)
1200.	-165.443	-171.826	-178.351	-185.024	(-191.847)	(-198.828)	(-205.971)	(-213.282)	(-220.766)
1250.	-160.625	-167.109	-173.737	-180.514	-187.446	(-194.536)	(-201.791)	(-209.218)	(-216.820)
1300.	-155.971	-162.556	-169.287	-176.169	-183.208	(-190.408)	(-197.777)	(-205.318)	(-213.038)
1350.	-151.469	-158.155	-164.989	-171.976	-179.122	-186.433	(-193.913)	(-201.570)	(-209.409)
1400.	-147.109	-153.895	-160.831	-167.924	-175.178	-182.598	(-190.191)	(-197.963)	(-205.920)
1450.	-142.879	-149.765	-156.805	-164.003	-171.364	-178.894	(-186.600)	(-194.487)	(-202.562)
1500.	-138.771	-145.758	-152.901	-160.204	-167.672	-175.313	-183.131	(-191.133)	(-199.326)
1550.	-134.778	-141.865	-149.110	-156.519	-164.095	-171.845	-179.776	(-187.894)	(-196.204)
1600.	-130.891	-138.079	-145.427	-152.941	-160.624	-168.484	-176.528	-184.761	-193.189
1645.	-127.479	-134.758	-142.198	-149.806	-157.587	-165.546	-173.691	-182.027	-190.561
1650.	-127.104	-134.393	-141.844	-149.463	-157.254	-165.224	-173.380	-181.728	-190.274
1665.	(-125.987)	(-133.306)	-140.788	-148.438	-156.261	-164.265	-172.454	-180.837	-189.418
1665.	(-125.987)	(-133.306)	-140.788	-148.438	-156.261	-164.265	-172.454	-180.837	-189.418
1697.15	(-123.620)	(-131.004)	(-138.552)	(-146.269)	(-154.162)	(-162.236)	(-170.498)	(-178.955)	(-187.612)
1700.	(-123.412)	(-130.802)	(-138.355)	(-146.079)	(-153.978)	(-162.058)	(-170.327)	(-178.790)	(-187.454)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.16. The function $\overline{H}(O_2)-\overline{H}^\circ(O_2)$, J/(mol K), in wustite, $Fe_{1-y}O$, for y = 0 to y = 0.16 between 800 and 1700 K at one bar total presure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the function for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
800.	(-592807.)	(-593351.)	(-593906.)	(-594473.)	(-595052.)	(-595643.)	(-596247.)	(-596863.)	(-597493.)
825.	(-589688.)	(-590267.)	(-590858.)	(-591461.)	(-592076.)	(-592705.)	(-593347.)	(-594002.)	(-594672.)
839.15	(-587915.)	(-588514.)	(-589126.)	(-589749.)	(-590386.)	(-591037.)	(-591701.)	(-592379.)	(-593072.)
850.	(-586553.)	(-587167.)	(-587794.)	(-588434.)	(-589088.)	(-589755.)	(-590436.)	(-591132.)	(-591843.)
875.	(-583400.)	(-584051.)	(-584716.)	(-585394.)	(-586087.)	(-586793.)	(-587515.)	(-588253.)	-589007.
900.	(-580231.)	(-580920.)	(-581623.)	(-582340.)	(-583073.)	(-583821.)	(-584584.)	(-585365.)	-586162.
925.	(-577044.)	(-577772.)	(-578515.)	(-579273.)	(-580046.)	(-580836.)	(-581643.)	-582467.	-583310.
950.	(-573841.)	(-574608.)	(-575392.)	(-576191.)	(-577007.)	(-577841.)	(-578692.)	-579561.	-580449.
1000.	(-567382.)	(-568233.)	(-569101.)	(-569987.)	(-570891.)	(-571815.)	-572758.	-573721.	-574705.
1050.	(-560856.)	(-561794.)	(-562751.)	(-563728.)	(-564725.)	(-565743.)	-566782.	-567845.	-568930.
1100.	(-554262.)	(-555291.)	(-556342.)	(-557414.)	(-558508.)	(-559625.)	-560766.	-561932.	-563123.
1150.	(-547600.)	(-548725.)	(-549873.)	(-551044.)	(-552240.)	-553462.	-554709.	-555983.	-557284.
1184.	(-543031.)	(-544223.)	(-545440.)	(-546682.)	(-547950.)	-549244.	-550566.	-551917.	-553296.
1184.	(-543031.)	(-544223.)	(-545440.)	(-546682.)	(-547950.)	-549244.	-550566.	-551917.	-553296.
1200.	(-540870.)	(-542095.)	(-543345.)	(-544620.)	(-545922.)	-547252.	-548610.	-549997.	-551415.
1250.	(-534071.)	(-535401.)	(-536757.)	(-538141.)	(-539554.)	-540997.	-542470.	-543975.	-545513.
1300.	(-527205.)	(-528643.)	(-530110.)	(-531607.)	(-533135.)	-534696.	-536289.	-537917.	-539581.
1350.	(-520271.)	(-521821.)	(-523403.)	(-525018.)	(-526666.)	-528349.	-530067.	-531823.	-533617.
1400.	(-513268.)	(-514936.)	(-516637.)	(-518373.)	(-520146.)	-521956.	-523804.	-525692.	-527621.
1450.	(-506198.)	(-507986.)	(-509811.)	(-511674.)	(-513575.)	-515517.	-517499.	-519525.	-521594.
1500.	(-499060.)	(-500974.)	(-502926.)	(-504920.)	(-506954.)	-509032.	-511154.	-513321.	-515536.
1550.	(-491853.)	(-493897.)	(-495982.)	(-498110.)	(-500283.)	-502502.	-504767.	-507081.	-509446.
1600.	(-484579.)	(-486756.)	(-488978.)	(-491246.)	(-493561.)	-495925.	-498339.	-500805.	-503325.
1645.	(-477973.)	(-480275.)	(-482624.)	(-485021.)	(-487468.)	-489967.	-492519.	-495126.	-497789.
1650.	(-477236.)	(-479552.)	(-481915.)	(-484327.)	(-486789.)	(-489303.)	(-491870.)	-494493.	-497172.
1665.	(-475020.)	(-477378.)	(-479784.)	(-482240.)	(-484747.)	(-487307.)	(-489921.)	(-492592.)	(-495320.)
1665.	(-475020.)	(-477378.)	(-479784.)	(-482240.)	(-484747.)	(-487307.)	(-489921.)	(-492592.)	(-495320.)
1697.15	(-470250.)	(-472700.)	(-475200.)	(-477751.)	(-480356.)	(-483016.)	(-485732.)	(-488507.)	(-491342.)
1700.	(-469825.)	(-472284.)	(-474792.)	(-477352.)	(-479966.)	(-482635.)	(-485360.)	(-488144.)	(-490988.)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

Table 9.16 Continued. The function $\overline{H}(O_2)-\overline{H}^\circ(O_2)$, J/(mol K), in wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
800.	(-597493.)	(-598137.)	(-598795.)	(-599468.)	(-600156.)	(-600860.)	(-601580.)	(-602318.)	(-603072.)
825.	(-594672.)	(-595357.)	(-596057.)	(-596772.)	(-597504.)	(-598253.)	(-599019.)	(-599803.)	(-600606.)
839.15	(-593072.)	(-593780.)	(-594504.)	(-595245.)	(-596002.)	(-596776.)	(-597569.)	(-598380.)	(-599211.)
850.	(-591843.)	(-592570.)	(-593313.)	(-594073.)	(-594849.)	(-595644.)	(-596457.)	(-597290.)	(-598142.)
875.	-589007.	(-589777.)	(-590564.)	(-591369.)	(-592192.)	(-593034.)	(-593896.)	(-594778.)	(-595681.)
900.	-586162.	(-586977.)	(-587810.)	(-588661.)	(-589532.)	(-590423.)	(-591335.)	(-592268.)	(-593223.)
925.	-583310.	-584170.	(-585050.)	(-585950.)	(-586870.)	(-587811.)	(-588774.)	(-589759.)	(-590769.)
950.	-580449.	-581357.	(-582285.)	(-583234.)	(-584204.)	(-585197.)	(-586213.)	(-587253.)	(-588317.)
1000.	-574705.	-575711.	(-576739.)	(-577791.)	(-578866.)	(-579966.)	(-581091.)	(-582243.)	(-583423.)
1050.	-568930.	-570039.	-571172.	(-572331.)	(-573517.)	(-574729.)	(-575970.)	(-577241.)	(-578541.)
1100.	-563123.	-564340.	-565584.	(-566856.)	(-568157.)	(-569488.)	(-570850.)	(-572244.)	(-573671.)
1150.	-557284.	-558615.	-559974.	-561365.	(-562787.)	(-564241.)	(-565730.)	(-567254.)	(-568813.)
1184.	-553296.	-554706.	-556148.	-557622.	(-559129.)	(-560671.)	(-562249.)	(-563864.)	(-565517.)
1184.	-553296.	-554706.	-556148.	-557622.	(-559129.)	(-560671.)	(-562249.)	(-563864.)	(-565517.)
1200.	-551415.	-552863.	-554344.	-555858.	(-557406.)	(-558990.)	(-560611.)	(-562269.)	(-563968.)
1250.	-545513.	-547085.	-548692.	-550334.	-552014.	(-553733.)	(-555492.)	(-557292.)	(-559134.)
1300.	-539581.	-541281.	-543018.	-544795.	-546612.	(-548471.)	(-550373.)	(-552320.)	(-554313.)
1350.	-533617.	-535450.	-537324.	-539240.	-541199.	-543204.	(-545255.)	(-547355.)	(-549504.)
1400.	-527621.	-529593.	-531608.	-533669.	-535776.	-537932.	(-540138.)	(-542396.)	(-544708.)
1450.	-521594.	-523709.	-525871.	-528081.	-530342.	-532655.	(-535021.)	(-537443.)	(-539923.)
1500.	-515536.	-517799.	-520113.	-522478.	-524897.	-527372.	-529905.	(-532497.)	(-535150.)
1550.	-509446.	-511863.	-514333.	-516859.	-519442.	-522085.	-524789.	(-527557.)	(-530390.)
1600.	-503325.	-505900.	-508532.	-511224.	-513976.	-516792.	-519673.	-522623.	-525642.
1645.	-497789.	-500511.	-503293.	-506138.	-509048.	-512024.	-515070.	-518187.	-521379.
1650.	-497172.	-499911.	-502710.	-505573.	-508500.	-511494.	-514559.	-517695.	-520906.
1665.	(-495320.)	(-498109.)	-500959.	-503874.	-506855.	-509904.	-513024.	-516218.	-519487.
1665.	(-495320.)	(-498109.)	-500959.	-503874.	-506855.	-509904.	-513024.	-516218.	-519487.
1697.15	(-491342.)	(-494239.)	(-497200.)	(-500229.)	(-503326.)	(-506494.)	(-509736.)	(-513054.)	(-516451.)
1700.	(-490988.)	(-493895.)	(-496867.)	(-499905.)	(-503013.)	(-506191.)	(-509444.)	(-512774.)	(-516182.)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.17. The function $\overline{G}(O_2)-\overline{G}^\circ(O_2)$, J/(mol K), in wustite, $Fe_{1-y}O$, for y = 0 to y = 0.16 between 800 and 1700 K at one bar total presure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the function for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
800.	(-455632.)	(-452402.)	(-449106.)	(-445743.)	(-442309.)	(-438803.)	(-435222.)	(-431565.)	(-427827.)
825.	(-451393.)	(-448045.)	(-444629.)	(-441141.)	(-437582.)	(-433947.)	(-430235.)	(-426443.)	(-422569.)
839.15	(-449037.)	(-445621.)	(-442135.)	(-438578.)	(-434946.)	(-431238.)	(-427451.)	(-423583.)	(-419631.)
850.	(-447250.)	(-443782.)	(-440243.)	(-436632.)	(-432945.)	(-429180.)	(-425336.)	(-421409.)	(-417396.)
875.	(-443198.)	(-439610.)	(-435948.)	(-432211.)	(-428396.)	(-424501.)	(-420523.)	(-416459.)	-412307.
900.	(-439237.)	(-435527.)	(-431742.)	(-427878.)	(-423933.)	(-419906.)	(-415793.)	(-411591.)	-407298.
925.	(-435365.)	(-431532.)	(-427621.)	(-423629.)	(-419554.)	(-415394.)	(-411145.)	-406804.	-402369.
950.	(-431578.)	(-427622.)	(-423584.)	(-419464.)	(-415257.)	(-410962.)	(-406576.)	-402095.	-397517.
1000.	(-424258.)	(-420050.)	(-415757.)	(-411375.)	(-406902.)	(-402335.)	-397671.	-392906.	-388038.
1050.	(-417262.)	(-412799.)	(-408246.)	(-403598.)	(-398854.)	(-394010.)	-389063.	-384009.	-378846.
1100.	(-410578.)	(-405857.)	(-401038.)	(-396121.)	(-391101.)	(-385976.)	-380741.	-375394.	-369930.
1150.	(-404196.)	(-399211.)	(-394124.)	(-388932.)	(-383632.)	-378220.	-372694.	-367048.	-361280.
1184.	(-400023.)	(-394856.)	(-389584.)	(-384203.)	(-378710.)	-373101.	-367373.	-361522.	-355543.
1184.	(-400023.)	(-394856.)	(-389584.)	(-384203.)	(-378710.)	-373101.	-367373.	-361522.	-355543.
1200.	(-398105.)	(-392852.)	(-387492.)	(-382021.)	(-376436.)	-370734.	-364910.	-358962.	-352883.
1250.	(-392296.)	(-386771.)	(-381133.)	(-375379.)	(-369505.)	-363507.	-357382.	-351125.	-344732.
1300.	(-386760.)	(-380959.)	(-375039.)	(-368997.)	(-362830.)	-356532.	-350101.	-343531.	-336818.
1350.	(-381490.)	(-375408.)	(-369202.)	(-362868.)	(-356402.)	-349800.	-343058.	-336170.	-329133.
1400.	(-376478.)	(-370111.)	(-363615.)	(-356984.)	(-350215.)	-343304.	-336246.	-329036.	-321669.
1450.	(-371717.)	(-365061.)	(-358270.)	(-351338.)	(-344262.)	-337037.	-329658.	-322121.	-314420.
1500.	(-367201.)	(-360252.)	(-353161.)	(-345924.)	(-338536.)	-330993.	-323289.	-315420.	-307379.
1550.	(-362925.)	(-355678.)	(-348283.)	(-340737.)	(-333032.)	-325166.	-317132.	-308926.	-300541.
1600.	(-358882.)	(-351333.)	(-343631.)	(-335769.)	(-327744.)	-319550.	-311182.	-302634.	-293899.
1645.	(-355438.)	(-347615.)	(-339631.)	(-331483.)	(-323165.)	-314673.	-305999.	-297139.	-288086.
1650.	(-355067.)	(-347212.)	(-339198.)	(-331018.)	(-322667.)	(-314141.)	(-305433.)	-296538.	-287450.
1665.	(-353966.)	(-346019.)	(-337910.)	(-329633.)	(-321184.)	(-312557.)	(-303747.)	(-294747.)	(-285552.)
1665.	(-353966.)	(-346019.)	(-337910.)	(-329633.)	(-321184.)	(-312557.)	(-303747.)	(-294747.)	(-285552.)
1697.15	(-351675.)	(-343528.)	(-335214.)	(-326730.)	(-318068.)	(-309224.)	(-300192.)	(-290966.)	(-281539.)
1700.	(-351476.)	(-343311.)	(-334979.)	(-326476.)	(-317796.)	(-308933.)	(-299881.)	(-290635.)	(-281187.)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

Table 9.17 Continued. The function $\overline{G}\backslash O_2)-\overline{G}^\circ(O_2)$, J/(mol K), in wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
800.	(-427827.)	(-424008.)	(-420104.)	(-416112.)	(-412029.)	(-407853.)	(-403579.)	(-399205.)	(-394727.)
825.	(-422569.)	(-418610.)	(-414562.)	(-410424.)	(-406191.)	(-401862.)	(-397431.)	(-392897.)	(-388254.)
839.15	(-419631.)	(-415592.)	(-411463.)	(-407241.)	(-402923.)	(-398506.)	(-393986.)	(-389360.)	(-384624.)
850.	(-417396.)	(-413295.)	(-409104.)	(-404817.)	(-400434.)	(-395950.)	(-391361.)	(-386664.)	(-381856.)
875.	-412307.	(-408063.)	(-403726.)	(-399290.)	(-394754.)	(-390114.)	(-385366.)	(-380506.)	(-375531.)
900.	-407298.	(-402911.)	(-398426.)	(-393841.)	(-389151.)	(-384354.)	(-379444.)	(-374420.)	(-369276.)
925.	-402369.	-397837.	(-393204.)	(-388466.)	(-383621.)	(-378665.)	(-373594.)	(-368403.)	(-363089.)
950.	-397517.	-392838.	(-388056.)	(-383165.)	(-378164.)	(-373048.)	(-367812.)	(-362454.)	(-356968.)
1000.	-388038.	-383062.	(-377976.)	(-372776.)	(-367458.)	(-362017.)	(-356450.)	(-350752.)	(-344918.)
1050.	-378846.	-373569.	-368175.	(-362660.)	(-357019.)	(-351249.)	(-345344.)	(-339300.)	(-333113.)
1100.	-369930.	-364347.	-358640.	(-352803.)	(-346835.)	(-340730.)	(-334482.)	(-328087.)	(-321540.)
1150.	-361280.	-355385.	-349358.	-343197.	(-336895.)	(-330449.)	(-323852.)	(-317101.)	(-310189.)
1184.	-355543.	-349433.	-343188.	-336801.	(-330270.)	(-323589.)	(-316752.)	(-309755.)	(-302591.)
1184.	-355543.	-349433.	-343188.	-336801.	(-330270.)	(-323589.)	(-316752.)	(-309755.)	(-302591.)
1200.	-352883.	-346672.	-340322.	-333829.	(-327189.)	(-320397.)	(-313446.)	(-306331.)	(-299048.)
1250.	-344732.	-338199.	-331520.	-324691.	-317707.	(-310563.)	(-303252.)	(-295770.)	(-288109.)
1300.	-336818.	-329958.	-322945.	-315775.	-308442.	(-300940.)	(-293264.)	(-285407.)	(-277363.)
1350.	-329133.	-321941.	-314589.	-307072.	-299384.	-291520.	(-283472.)	(-275235.)	(-266803.)
1400.	-321669.	-314140.	-306444.	-298575.	-290527.	-282295.	(-273870.)	(-265248.)	(-256420.)
1450.	-314420.	-306549.	-298504.	-290277.	-281864.	-273258.	(-264451.)	(-255437.)	(-246209.)
1500.	-307379.	-299162.	-290762.	-282173.	-273389.	-264403.	-255208.	(-245797.)	(-236162.)
1550.	-300541.	-291971.	-283212.	-274255.	-265095.	-255725.	-246136.	(-236322.)	(-226274.)
1600.	-293899.	-284973.	-275849.	-266519.	-256977.	-247217.	-237229.	-227006.	-216540.
1645.	-288086.	-278835.	-269378.	-259707.	-249818.	-239702.	-229349.	-218753.	-207906.
1650.	-287450.	-278162.	-268667.	-258959.	-249031.	-238875.	-228481.	-217844.	-206954.
1665.	(-285552.)	(-276154.)	-266548.	-256725.	-246680.	-236404.	-225888.	-215125.	-204106.
1665.	(-285552.)	(-276154.)	-266548.	-256725.	-246680.	-236404.	-225888.	-215125.	-204106.
1697.15	(-281539.)	(-271905.)	(-262057.)	(-251988.)	(-241690.)	(-231155.)	(-220375.)	(-209341.)	(-198045.)
1700.	(-281187.)	(-271532.)	(-261663.)	(-251571.)	(-241250.)	(-230693.)	(-219889.)	(-208831.)	(-197511.)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.18. Activity of the O_2 component, log $a(O_2)$, in wustite, $Fe_{1-y}O$, for y = 0 to y = 0.16 between 800 and 1700 K at one bar total pressure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature.

Temperature (K)	Composition of Wustite: first line = "y", second line = "x" (moles)								
	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
	0.0000	0.0101	0.0204	0.0309	0.0417	0.0526	0.0638	0.0753	0.0870
800.	(-29.7514)	(-29.5405)	(-29.3253)	(-29.1057)	(-28.8815)	(-28.6526)	(-28.4188)	(-28.1800)	(-27.9360)
825.	(-28.5796)	(-28.3676)	(-28.1513)	(-27.9305)	(-27.7051)	(-27.4750)	(-27.2400)	(-26.9999)	(-26.7546)
839.15	(-27.9505)	(-27.7379)	(-27.5209)	(-27.2995)	(-27.0734)	(-26.8426)	(-26.6069)	(-26.3661)	(-26.1201)
850.	(-27.4837)	(-27.2706)	(-27.0532)	(-26.8312)	(-26.6047)	(-26.3734)	(-26.1371)	(-25.8958)	(-25.6492)
875.	(-26.4569)	(-26.2427)	(-26.0241)	(-25.8010)	(-25.5732)	(-25.3407)	(-25.1032)	(-24.8607)	-24.6128
900.	(-25.4929)	(-25.2776)	(-25.0579)	(-24.8337)	(-24.6047)	(-24.3710)	(-24.1323)	(-23.8884)	-23.6393
925.	(-24.5865)	(-24.3700)	(-24.1492)	(-23.9238)	(-23.6937)	(-23.4587)	(-23.2188)	-22.9737	-22.7233
950.	(-23.7326)	(-23.5151)	(-23.2931)	(-23.0665)	(-22.8353)	(-22.5991)	(-22.3580)	-22.1116	-21.8599
1000.	(-22.1658)	(-21.9461)	(-21.7218)	(-21.4929)	(-21.2593)	(-21.0207)	-20.7771	-20.5282	-20.2739
1050.	(-20.7619)	(-20.5400)	(-20.3134)	(-20.0823)	(-19.8462)	(-19.6053)	-19.3592	-19.1078	-18.8509
1100.	(-19.4978)	(-19.2736)	(-19.0448)	(-18.8113)	(-18.5729)	(-18.3295)	-18.0810	-17.8271	-17.5676
1150.	(-18.3570)	(-18.1305)	(-17.8995)	(-17.6637)	(-17.4230)	-17.1772	-16.9261	-16.6697	-16.4077
1184.	(-17.6438)	(-17.4159)	(-17.1833)	(-16.9459)	(-16.7036)	-16.4561	-16.2034	-15.9453	-15.6816
1184.	(-17.6438)	(-17.4159)	(-17.1833)	(-16.9459)	(-16.7036)	-16.4561	-16.2034	-15.9453	-15.6816
1200.	(-17.3256)	(-17.0970)	(-16.8636)	(-16.6255)	(-16.3824)	-16.1342	-15.8807	-15.6218	-15.3572
1250.	(-16.3912)	(-16.1604)	(-15.9248)	(-15.6843)	(-15.4389)	-15.1883	-14.9323	-14.6709	-14.4037
1300.	(-15.5394)	(-15.3064)	(-15.0685)	(-14.8257)	(-14.5779)	-14.3249	-14.0665	-13.8025	-13.5328
1350.	(-14.7608)	(-14.5254)	(-14.2853)	(-14.0402)	(-13.7901)	-13.5346	-13.2737	-13.0073	-12.7350
1400.	(-14.0470)	(-13.8095)	(-13.5671)	(-13.3197)	(-13.0672)	-12.8093	-12.5460	-12.2770	-12.0021
1450.	(-13.3913)	(-13.1515)	(-12.9069)	(-12.6572)	(-12.4023)	-12.1420	-11.8762	-11.6047	-11.3273
1500.	(-12.7876)	(-12.5456)	(-12.2987)	(-12.0467)	(-11.7894)	-11.5267	-11.2584	-10.9844	-10.7044
1550.	(-12.2306)	(-11.9864)	(-11.7372)	(-11.4829)	(-11.2233)	-10.9582	-10.6874	-10.4109	-10.1283
1600.	(-11.7159)	(-11.4694)	(-11.2180)	(-10.9613)	(-10.6993)	-10.4319	-10.1587	-9.8796	-9.5945
1645.	(-11.2854)	(-11.0370)	(-10.7834)	(-10.5247)	(-10.2606)	-9.9910	-9.7155	-9.4342	-9.1468
1650.	(-11.2393)	(-10.9907)	(-10.7370)	(-10.4780)	(-10.2137)	(-9.9438)	(-9.6681)	-9.3865	-9.0988
1665.	(-11.1033)	(-10.8540)	(-10.5996)	(-10.3399)	(-10.0749)	(-9.8043)	(-9.5279)	(-9.2455)	(-8.9570)
1665.	(-11.1033)	(-10.8540)	(-10.5996)	(-10.3399)	(-10.0749)	(-9.8042)	(-9.5278)	(-9.2455)	(-8.9570)
1697.15	(-10.8231)	(-10.5724)	(-10.3165)	(-10.0554)	(-9.7888)	(-9.5166)	(-9.2387)	(-8.9547)	(-8.6646)
1700.	(-10.7989)	(-10.5481)	(-10.2921)	(-10.0308)	(-9.7641)	(-9.4918)	(-9.2137)	(-8.9296)	(-8.6393)

Table 9.18 Continued. Activity of the O_2 component, log $a(O_2)$, in wustite, $Fe_{1-y}O$.

Temperature (K)	Composition of Wustite: first line = "y", second line = "x" (moles)								
	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
	0.0870	0.0999	0.1111	0.1236	0.1364	0.1494	0.1628	0.1765	0.1905
800.	(-27.9360)	(-27.6866)	(-27.4317)	(-27.1710)	(-26.9045)	(-26.6318)	(-26.3527)	(-26.0671)	(-25.7748)
825.	(-26.7546)	(-26.5040)	(-26.2477)	(-25.9857)	(-25.7177)	(-25.4436)	(-25.1631)	(-24.8760)	(-24.5821)
839.15	(-26.1201)	(-25.8687)	(-25.6117)	(-25.3489)	(-25.0801)	(-24.8052)	(-24.5238)	(-24.2359)	(-23.9411)
850.	(-25.6492)	(-25.3972)	(-25.1396)	(-24.8762)	(-24.6069)	(-24.3313)	(-24.0493)	(-23.7607)	(-23.4653)
875.	-24.6128	(-24.3595)	(-24.1006)	(-23.8358)	(-23.5650)	(-23.2880)	(-23.0046)	(-22.7144)	(-22.4175)
900.	-23.6393	(-23.3847)	(-23.1244)	(-22.8582)	(-22.5861)	(-22.3076)	(-22.0227)	(-21.7311)	(-21.4326)
925.	-22.7233	-22.4673	(-22.2057)	(-21.9382)	(-21.6646)	(-21.3847)	(-21.0984)	(-20.8052)	(-20.5051)
950.	-21.8599	-21.6026	(-21.3396)	(-21.0708)	(-20.7958)	(-20.5145)	(-20.2266)	(-19.9320)	(-19.6304)
1000.	-20.2739	-20.0141	(-19.7484)	(-19.4768)	(-19.1990)	(-18.9148)	(-18.6240)	(-18.3264)	(-18.0217)
1050.	-18.8509	-18.5884	-18.3201	(-18.0457)	(-17.7651)	(-17.4781)	(-17.1843)	(-16.8837)	(-16.5759)
1100.	-17.5676	-17.3025	-17.0315	(-16.7544)	(-16.4710)	(-16.1810)	(-15.8843)	(-15.5807)	(-15.2698)
1150.	-16.4077	-16.1399	-15.8662	-15.5864	(-15.3001)	(-15.0074)	(-14.7078)	(-14.4011)	(-14.0871)
1184.	-15.6816	-15.4120	-15.1365	-14.8547	(-14.5666)	(-14.2719)	(-13.9703)	(-13.6616)	(-13.3455)
1184.	-15.6816	-15.4120	-15.1365	-14.8547	(-14.5666)	(-14.2719)	(-13.9703)	(-13.6616)	(-13.3455)
1200.	-15.3572	-15.0868	-14.8104	-14.5278	(-14.2388)	(-13.9431)	(-13.6406)	(-13.3309)	(-13.0139)
1250.	-14.4037	-14.1307	-13.8516	-13.5663	-13.2744	(-12.9759)	(-12.6704)	(-12.3577)	(-12.0376)
1300.	-13.5328	-13.2572	-12.9754	-12.6873	-12.3926	(-12.0913)	(-11.7828)	(-11.4671)	(-11.1439)
1350.	-12.7350	-12.4567	-12.1723	-11.8814	-11.5840	-11.2797	(-10.9683)	(-10.6496)	(-10.3234)
1400.	-12.0021	-11.7212	-11.4341	-11.1405	-10.8402	-10.5331	(-10.2188)	(-9.8971)	(-9.5677)
1450.	-11.3273	-11.0438	-10.7539	-10.4576	-10.1545	-9.8445	(-9.5272)	(-9.2025)	(-8.8701)
1500.	-10.7044	-10.4183	-10.1258	-9.8267	-9.5208	-9.2079	-8.8877	(-8.5600)	(-8.2245)
1550.	-10.1283	-9.8396	-9.5444	-9.2425	-8.9338	-8.6181	-8.2949	(-7.9642)	(-7.6256)
1600.	-9.5945	-9.3031	-9.0052	-8.7006	-8.3891	-8.0705	-7.7444	-7.4107	-7.0690
1645.	-9.1468	-8.8530	-8.5527	-8.2457	-7.9316	-7.6104	-7.2817	-6.9452	-6.6008
1650.	-9.0988	-8.8048	-8.5042	-8.1969	-7.8826	-7.5611	-7.2321	-6.8953	-6.5506
1665.	(-8.9570)	(-8.6622)	-8.3609	-8.0527	-7.7376	-7.4152	-7.0853	-6.7477	-6.4020
1665.	(-8.9570)	(-8.6622)	-8.3608	-8.0527	-7.7376	-7.4152	-7.0853	-6.7476	-6.4020
1697.15	(-8.6646)	(-8.3681)	(-8.0650)	(-7.7551)	(-7.4381)	(-7.1139)	(-6.7821)	(-6.4425)	(-6.0949)
1700.	(-8.6393)	(-8.3426)	(-8.0394)	(-7.7293)	(-7.4122)	(-7.0878)	(-6.7559)	(-6.4161)	(-6.0683)

Table 9.19. The function $\bar{S}$(FeO)-$\bar{S}$°(FeO), J/(mol K), in wustite, $Fe_{1-y}O$, for y = 0 to y = 0.16 between 800 and 1700 K at one bar total presure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the function for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
800.	(0.000)	(0.012)	(0.049)	(0.112)	(0.203)	(0.323)	(0.476)	(0.662)	(0.883)
825.	(0.000)	(0.012)	(0.049)	(0.113)	(0.205)	(0.326)	(0.480)	(0.667)	(0.891)
839.15	(0.000)	(0.012)	(0.049)	(0.113)	(0.206)	(0.328)	(0.482)	(0.671)	(0.895)
850.	(0.000)	(0.012)	(0.050)	(0.114)	(0.206)	(0.329)	(0.484)	(0.673)	(0.899)
875.	(0.000)	(0.012)	(0.050)	(0.115)	(0.208)	(0.332)	(0.489)	(0.679)	0.907
900.	(0.000)	(0.012)	(0.050)	(0.116)	(0.210)	(0.335)	(0.493)	(0.685)	0.915
925.	(0.000)	(0.012)	(0.051)	(0.117)	(0.212)	(0.338)	(0.497)	0.691	0.923
950.	(0.000)	(0.013)	(0.051)	(0.118)	(0.214)	(0.341)	(0.501)	0.697	0.931
1000.	(0.000)	(0.013)	(0.052)	(0.120)	(0.217)	(0.347)	0.510	0.709	0.947
1050.	(0.000)	(0.013)	(0.053)	(0.122)	(0.221)	(0.353)	0.519	0.721	0.963
1100.	(0.000)	(0.013)	(0.054)	(0.124)	(0.225)	(0.358)	0.527	0.733	0.978
1150.	(0.000)	(0.013)	(0.055)	(0.126)	(0.228)	0.364	0.536	0.745	0.994
1184.	(0.000)	(0.014)	(0.055)	(0.127)	(0.231)	0.368	0.542	0.753	1.005
1184.	(0.000)	(0.014)	(0.055)	(0.127)	(0.231)	0.368	0.542	0.753	1.005
1200.	(0.000)	(0.014)	(0.056)	(0.128)	(0.232)	0.370	0.544	0.757	1.010
1250.	(0.000)	(0.014)	(0.057)	(0.130)	(0.236)	0.376	0.553	0.769	1.026
1300.	(0.000)	(0.014)	(0.057)	(0.132)	(0.239)	0.382	0.562	0.781	1.042
1350.	(0.000)	(0.014)	(0.058)	(0.134)	(0.243)	0.388	0.570	0.793	1.058
1400.	(0.000)	(0.014)	(0.059)	(0.136)	(0.247)	0.393	0.579	0.805	1.074
1450.	(0.000)	(0.015)	(0.060)	(0.138)	(0.250)	0.399	0.587	0.817	1.090
1500.	(0.000)	(0.015)	(0.061)	(0.140)	(0.254)	0.405	0.596	0.829	1.106
1550.	(0.000)	(0.015)	(0.062)	(0.142)	(0.258)	0.411	0.604	0.840	1.122
1600.	(0.000)	(0.015)	(0.063)	(0.144)	(0.261)	0.417	0.613	0.852	1.138
1645.	(0.000)	(0.016)	(0.063)	(0.146)	(0.264)	0.422	0.621	0.863	1.152
1650.	(0.000)	(0.016)	(0.064)	(0.146)	(0.265)	(0.423)	(0.622)	0.864	1.154
1665.	(0.000)	(0.016)	(0.064)	(0.147)	(0.266)	(0.424)	(0.624)	(0.868)	(1.158)
1665.	(0.000)	(0.016)	(0.064)	(0.147)	(0.266)	(0.424)	(0.624)	(0.868)	(1.158)
1697.15	(0.000)	(0.016)	(0.064)	(0.148)	(0.268)	(0.428)	(0.630)	(0.876)	(1.169)
1700.	(0.000)	(0.016)	(0.064)	(0.148)	(0.269)	(0.428)	(0.630)	(0.876)	(1.169)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

Table 9.19 Continued. The function $\bar{S}$(FeO)-$\bar{S}$°(FeO), J/(mol K), in wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
800.	(0.883)	(1.142)	(1.442)	(1.784)	(2.171)	(2.607)	(3.094)	(3.636)	(4.236)
825.	(0.891)	(1.152)	(1.455)	(1.800)	(2.191)	(2.631)	(3.122)	(3.669)	(4.275)
839.15	(0.895)	(1.158)	(1.462)	(1.809)	(2.202)	(2.644)	(3.138)	(3.688)	(4.296)
850.	(0.899)	(1.163)	(1.468)	(1.816)	(2.210)	(2.654)	(3.150)	(3.702)	(4.313)
875.	0.907	(1.173)	(1.481)	(1.832)	(2.230)	(2.678)	(3.178)	(3.735)	(4.351)
900.	0.915	(1.183)	(1.494)	(1.848)	(2.250)	(2.701)	(3.206)	(3.767)	(4.389)
925.	0.923	1.194	(1.507)	(1.864)	(2.269)	(2.725)	(3.234)	(3.800)	(4.427)
950.	0.931	1.204	(1.520)	(1.880)	(2.289)	(2.748)	(3.262)	(3.833)	(4.466)
1000.	0.947	1.225	(1.546)	(1.912)	(2.328)	(2.795)	(3.318)	(3.899)	(4.542)
1050.	0.963	1.245	1.571	(1.945)	(2.367)	(2.842)	(3.373)	(3.964)	(4.618)
1100.	0.978	1.266	1.597	(1.977)	(2.406)	(2.889)	(3.429)	(4.030)	(4.695)
1150.	0.994	1.286	1.623	2.009	(2.445)	(2.936)	(3.485)	(4.095)	(4.771)
1184.	1.005	1.300	1.641	2.031	(2.472)	(2.968)	(3.523)	(4.140)	(4.823)
1184.	1.005	1.300	1.641	2.031	(2.472)	(2.968)	(3.523)	(4.140)	(4.823)
1200.	1.010	1.307	1.649	2.041	(2.484)	(2.983)	(3.541)	(4.161)	(4.847)
1250.	1.026	1.327	1.675	2.073	2.524	(3.030)	(3.596)	(4.226)	(4.924)
1300.	1.042	1.348	1.701	2.105	2.563	(3.077)	(3.652)	(4.292)	(5.000)
1350.	1.058	1.369	1.727	2.137	2.602	3.124	(3.708)	(4.357)	(5.077)
1400.	1.074	1.389	1.753	2.170	2.641	3.171	(3.764)	(4.423)	(5.153)
1450.	1.090	1.410	1.779	2.202	2.680	3.218	(3.820)	(4.489)	(5.229)
1500.	1.106	1.430	1.805	2.234	2.719	3.265	3.875	(4.554)	(5.306)
1550.	1.122	1.451	1.831	2.266	2.758	3.312	3.931	(4.620)	(5.382)
1600.	1.138	1.472	1.857	2.298	2.798	3.359	3.987	4.685	5.458
1645.	1.152	1.490	1.881	2.327	2.833	3.402	4.037	4.744	5.527
1650.	1.154	1.492	1.883	2.330	2.837	3.406	4.043	4.751	5.535
1665.	(1.158)	(1.498)	1.891	2.340	2.849	3.420	4.060	4.771	5.558
1665.	(1.158)	(1.498)	1.891	2.340	2.849	3.420	4.060	4.771	5.558
1697.15	(1.169)	(1.512)	(1.908)	(2.361)	(2.874)	(3.451)	(4.095)	(4.813)	(5.607)
1700.	(1.169)	(1.513)	(1.909)	(2.363)	(2.876)	(3.453)	(4.099)	(4.816)	(5.611)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.20. The function $\overline{H}(FeO)-\overline{H}^{\circ}(FeO)$, J/(mol K), in wustite, $Fe_{1-y}O$, for y = 0 to y = 0.16 between 800 and 1700 K at one bar total presure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the function for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
800.	(0.)	(1.)	(6.)	(13.)	(23.)	(37.)	(55.)	(76.)	(102.)
825.	(0.)	(1.)	(6.)	(14.)	(25.)	(40.)	(58.)	(81.)	(108.)
839.15	(0.)	(2.)	(6.)	(14.)	(26.)	(41.)	(60.)	(84.)	(112.)
850.	(0.)	(2.)	(6.)	(15.)	(26.)	(42.)	(62.)	(86.)	(115.)
875.	(0.)	(2.)	(7.)	(15.)	(28.)	(45.)	(66.)	(91.)	122.
900.	(0.)	(2.)	(7.)	(16.)	(30.)	(47.)	(69.)	(97.)	129.
925.	(0.)	(2.)	(8.)	(17.)	(31.)	(50.)	(73.)	102.	136.
950.	(0.)	(2.)	(8.)	(18.)	(33.)	(53.)	(77.)	108.	144.
1000.	(0.)	(2.)	(9.)	(20.)	(37.)	(58.)	86.	119.	159.
1050.	(0.)	(2.)	(10.)	(22.)	(40.)	(64.)	95.	131.	176.
1100.	(0.)	(3.)	(11.)	(24.)	(44.)	(71.)	104.	144.	193.
1150.	(0.)	(3.)	(12.)	(27.)	(48.)	77.	113.	158.	211.
1184.	(0.)	(3.)	(12.)	(28.)	(51.)	82.	120.	167.	223.
1184.	(0.)	(3.)	(12.)	(28.)	(51.)	82.	120.	167.	223.
1200.	(0.)	(3.)	(13.)	(29.)	(53.)	84.	124.	172.	229.
1250.	(0.)	(3.)	(14.)	(31.)	(57.)	91.	134.	186.	249.
1300.	(0.)	(4.)	(15.)	(34.)	(62.)	99.	145.	202.	269.
1350.	(0.)	(4.)	(16.)	(37.)	(67.)	106.	156.	217.	290.
1400.	(0.)	(4.)	(17.)	(39.)	(72.)	114.	168.	234.	312.
1450.	(0.)	(5.)	(18.)	(42.)	(77.)	123.	180.	251.	335.
1500.	(0.)	(5.)	(20.)	(45.)	(82.)	131.	193.	268.	358.
1550.	(0.)	(5.)	(21.)	(48.)	(88.)	140.	206.	287.	382.
1600.	(0.)	(5.)	(22.)	(52.)	(94.)	149.	220.	305.	408.
1645.	(0.)	(6.)	(24.)	(54.)	(99.)	158.	232.	323.	431.
1650.	(0.)	(6.)	(24.)	(55.)	(100.)	(159.)	(234.)	325.	433.
1665.	(0.)	(6.)	(24.)	(56.)	(101.)	(162.)	(238.)	(331.)	(441.)
1665.	(0.)	(6.)	(24.)	(56.)	(101.)	(162.)	(238.)	(331.)	(441.)
1697.15	(0.)	(6.)	(25.)	(58.)	(105.)	(168.)	(247.)	(344.)	(459.)
1700.	(0.)	(6.)	(25.)	(58.)	(106.)	(169.)	(248.)	(345.)	(460.)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

Table 9.20 Continued. The function $\overline{H}(FeO)-\overline{H}^{\circ}(FeO)$, J/(mol K), in wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
800.	(102.)	(132.)	(166.)	(206.)	(251.)	(301.)	(357.)	(420.)	(489.)
825.	(108.)	(140.)	(177.)	(219.)	(266.)	(320.)	(380.)	(446.)	(520.)
839.15	(112.)	(145.)	(183.)	(226.)	(276.)	(331.)	(393.)	(462.)	(538.)
850.	(115.)	(149.)	(188.)	(232.)	(283.)	(340.)	(403.)	(474.)	(552.)
875.	122.	(158.)	(199.)	(246.)	(300.)	(360.)	(427.)	(502.)	(585.)
900.	129.	(167.)	(211.)	(261.)	(317.)	(381.)	(452.)	(531.)	(619.)
925.	136.	176.	(222.)	(275.)	(335.)	(402.)	(477.)	(561.)	(654.)
950.	144.	186.	(235.)	(290.)	(353.)	(424.)	(504.)	(592.)	(689.)
1000.	159.	206.	(260.)	(322.)	(391.)	(470.)	(558.)	(656.)	(764.)
1050.	176.	227.	287.	(355.)	(432.)	(518.)	(615.)	(723.)	(842.)
1100.	193.	249.	314.	(389.)	(474.)	(569.)	(675.)	(793.)	(924.)
1150.	211.	272.	344.	425.	(518.)	(622.)	(738.)	(867.)	(1010.)
1184.	223.	289.	364.	451.	(549.)	(659.)	(782.)	(919.)	(1071.)
1184.	223.	289.	364.	451.	(549.)	(659.)	(782.)	(919.)	(1071.)
1200.	229.	297.	374.	463.	(564.)	(677.)	(803.)	(944.)	(1100.)
1250.	249.	322.	406.	503.	612.	(734.)	(872.)	(1024.)	(1193.)
1300.	269.	348.	439.	544.	662.	(794.)	(943.)	(1108.)	(1291.)
1350.	290.	375.	474.	586.	713.	857.	(1017.)	(1195.)	(1392.)
1400.	312.	404.	509.	630.	767.	921.	(1094.)	(1285.)	(1497.)
1450.	335.	433.	546.	676.	823.	988.	(1173.)	(1378.)	(1606.)
1500.	358.	463.	585.	724.	881.	1058.	1255.	(1475.)	(1719.)
1550.	382.	495.	624.	773.	941.	1129.	1340.	(1575.)	(1835.)
1600.	408.	527.	665.	823.	1002.	1203.	1428.	1678.	1955.
1645.	431.	557.	703.	870.	1059.	1272.	1510.	1774.	2067.
1650.	433.	561.	708.	876.	1066.	1280.	1519.	1785.	2080.
1665.	(441.)	(571.)	721.	892.	1085.	1303.	1547.	1818.	2117.
1665.	(441.)	(571.)	721.	892.	1085.	1303.	1547.	1818.	2117.
1697.15	(459.)	(593.)	(749.)	(926.)	(1128.)	(1354.)	(1607.)	(1888.)	(2200.)
1700.	(460.)	(595.)	(751.)	(929.)	(1131.)	(1358.)	(1612.)	(1895.)	(2207.)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.21. The function $\overline{G}(FeO)-\overline{G}^{\circ}(FeO)$, J/(mol K), in wustite, $Fe_{1-y}O$, for y = 0 to y = 0.16 between 800 and 1700 K at one bar total presure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature. To obtain the function for the formula FeO_{1+x}, multiply the tabulated value by the constant "1+x" as given at the bottom of each column.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
800.	(0.)	(-8.)	(-33.)	(-76.)	(-139.)	(-221.)	(-326.)	(-453.)	(-604.)
825.	(0.)	(-8.)	(-35.)	(-79.)	(-144.)	(-230.)	(-338.)	(-469.)	(-627.)
839.15	(0.)	(-9.)	(-35.)	(-81.)	(-147.)	(-234.)	(-344.)	(-479.)	(-639.)
850.	(0.)	(-9.)	(-36.)	(-82.)	(-149.)	(-238.)	(-350.)	(-486.)	(-649.)
875.	(0.)	(-9.)	(-37.)	(-85.)	(-154.)	(-246.)	(-362.)	(-503.)	-672.
900.	(0.)	(-9.)	(-38.)	(-88.)	(-159.)	(-254.)	(-374.)	(-520.)	-694.
925.	(0.)	(-10.)	(-40.)	(-91.)	(-165.)	(-263.)	(-386.)	-537.	-717.
950.	(0.)	(-10.)	(-41.)	(-94.)	(-170.)	(-271.)	(-399.)	-555.	-740.
1000.	(0.)	(-11.)	(-43.)	(-100.)	(-181.)	(-288.)	-424.	-590.	-787.
1050.	(0.)	(-11.)	(-46.)	(-106.)	(-192.)	(-306.)	-450.	-626.	-835.
1100.	(0.)	(-12.)	(-49.)	(-112.)	(-203.)	(-324.)	-476.	-662.	-884.
1150.	(0.)	(-13.)	(-51.)	(-118.)	(-214.)	-342.	-503.	-699.	-933.
1184.	(0.)	(-13.)	(-53.)	(-122.)	(-222.)	-354.	-521.	-724.	-967.
1184.	(0.)	(-13.)	(-53.)	(-122.)	(-222.)	-354.	-521.	-724.	-967.
1200.	(0.)	(-13.)	(-54.)	(-124.)	(-226.)	-360.	-530.	-737.	-983.
1250.	(0.)	(-14.)	(-57.)	(-131.)	(-237.)	-379.	-557.	-775.	-1034.
1300.	(0.)	(-15.)	(-60.)	(-137.)	(-249.)	-398.	-585.	-813.	-1086.
1350.	(0.)	(-15.)	(-63.)	(-144.)	(-261.)	-417.	-613.	-853.	-1138.
1400.	(0.)	(-16.)	(-66.)	(-151.)	(-274.)	-436.	-642.	-893.	-1192.
1450.	(0.)	(-17.)	(-69.)	(-158.)	(-286.)	-456.	-671.	-933.	-1246.
1500.	(0.)	(-18.)	(-72.)	(-165.)	(-299.)	-476.	-701.	-974.	-1300.
1550.	(0.)	(-18.)	(-75.)	(-172.)	(-311.)	-497.	-731.	-1016.	-1356.
1600.	(0.)	(-19.)	(-78.)	(-179.)	(-324.)	-518.	-761.	-1058.	-1413.
1645.	(0.)	(-20.)	(-81.)	(-185.)	(-336.)	-536.	-789.	-1097.	-1464.
1650.	(0.)	(-20.)	(-81.)	(-186.)	(-337.)	(-539.)	(-792.)	-1101.	-1470.
1665.	(0.)	(-20.)	(-82.)	(-188.)	(-341.)	(-545.)	(-801.)	(-1114.)	(-1487.)
1665.	(0.)	(-20.)	(-82.)	(-188.)	(-341.)	(-545.)	(-801.)	(-1114.)	(-1487.)
1697.15	(0.)	(-21.)	(-84.)	(-193.)	(-350.)	(-559.)	(-822.)	(-1142.)	(-1525.)
1700.	(0.)	(-21.)	(-84.)	(-193.)	(-351.)	(-560.)	(-823.)	(-1145.)	(-1528.)
"1+x" =	1.0000	1.0101	1.0204	1.0309	1.0417	1.0526	1.0638	1.0753	1.0870

Table 9.21 Continued. The function $\overline{G}(FeO)-\overline{G}^{\circ}(FeO)$, J/(mol K), in wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite as "y" (moles)								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
800.	(-604.)	(-782.)	(-987.)	(-1221.)	(-1486.)	(-1785.)	(-2118.)	(-2489.)	(-2900.)
825.	(-627.)	(-811.)	(-1023.)	(-1266.)	(-1541.)	(-1850.)	(-2196.)	(-2581.)	(-3007.)
839.15	(-639.)	(-827.)	(-1044.)	(-1291.)	(-1572.)	(-1888.)	(-2240.)	(-2633.)	(-3067.)
850.	(-649.)	(-840.)	(-1060.)	(-1311.)	(-1596.)	(-1916.)	(-2275.)	(-2673.)	(-3114.)
875.	-672.	(-869.)	(-1096.)	(-1357.)	(-1652.)	(-1983.)	(-2354.)	(-2766.)	(-3222.)
900.	-694.	(-898.)	(-1134.)	(-1403.)	(-1708.)	(-2050.)	(-2433.)	(-2860.)	(-3332.)
925.	-717.	-928.	(-1171.)	(-1449.)	(-1764.)	(-2118.)	(-2514.)	(-2954.)	(-3442.)
950.	-740.	-958.	(-1209.)	(-1496.)	(-1821.)	(-2186.)	(-2595.)	(-3050.)	(-3553.)
1000.	-787.	-1019.	(-1286.)	(-1591.)	(-1936.)	(-2325.)	(-2760.)	(-3243.)	(-3778.)
1050.	-835.	-1080.	-1364.	(-1687.)	(-2054.)	(-2466.)	(-2927.)	(-3439.)	(-4007.)
1100.	-884.	-1143.	-1443.	(-1785.)	(-2173.)	(-2609.)	(-3097.)	(-3639.)	(-4240.)
1150.	-933.	-1207.	-1523.	-1885.	(-2294.)	(-2755.)	(-3270.)	(-3842.)	(-4477.)
1184.	-967.	-1251.	-1579.	-1953.	(-2378.)	(-2855.)	(-3389.)	(-3982.)	(-4640.)
1184.	-967.	-1251.	-1579.	-1953.	(-2378.)	(-2855.)	(-3389.)	(-3982.)	(-4640.)
1200.	-983.	-1272.	-1605.	-1986.	(-2418.)	(-2903.)	(-3445.)	(-4049.)	(-4717.)
1250.	-1034.	-1338.	-1688.	-2089.	-2543.	(-3053.)	(-3624.)	(-4259.)	(-4961.)
1300.	-1086.	-1404.	-1773.	-2193.	-2670.	(-3206.)	(-3805.)	(-4471.)	(-5209.)
1350.	-1138.	-1472.	-1858.	-2299.	-2799.	-3361.	(-3989.)	(-4688.)	(-5461.)
1400.	-1192.	-1541.	-1945.	-2407.	-2930.	-3518.	(-4176.)	(-4907.)	(-5717.)
1450.	-1246.	-1611.	-2034.	-2516.	-3063.	-3678.	(-4366.)	(-5130.)	(-5977.)
1500.	-1300.	-1682.	-2123.	-2627.	-3198.	-3840.	-4558.	(-5356.)	(-6240.)
1550.	-1356.	-1754.	-2214.	-2740.	-3335.	-4005.	-4753.	(-5585.)	(-6507.)
1600.	-1413.	-1827.	-2306.	-2854.	-3474.	-4171.	-4951.	-5818.	-6778.
1645.	-1464.	-1894.	-2391.	-2958.	-3601.	-4323.	-5132.	-6030.	-7025.
1650.	-1470.	-1902.	-2400.	-2970.	-3615.	-4341.	-5152.	-6054.	-7053.
1665.	(-1487.)	(-1924.)	-2428.	-3005.	-3658.	-4392.	-5213.	-6125.	-7136.
1665.	(-1487.)	(-1924.)	-2428.	-3005.	-3658.	-4392.	-5213.	-6125.	-7136.
1697.15	(-1525.)	(-1972.)	(-2489.)	(-3080.)	(-3750.)	(-4502.)	(-5344.)	(-6279.)	(-7316.)
1700.	(-1528.)	(-1977.)	(-2495.)	(-3087.)	(-3758.)	(-4512.)	(-5355.)	(-6293.)	(-7332.)
"1+x" =	1.0870	1.0999	1.1111	1.1236	1.1364	1.1494	1.1628	1.1765	1.1905

Table 9.22. Activity of the FeO component, log a(FeO), in wustite, $Fe_{1-y}O$, for y = 0 to y = 0.16 between 800 and 1700 K at one bar total pressure. The data in parentheses are metastable at one bar total pressure. Refer to the text for the basis for extrapolating in composition and temperature.

Temperature	Composition of Wustite: first line = "y", second line = "x" (moles)								
(K)	0.0000	0.0100	0.0200	0.0300	0.0400	0.0500	0.0600	0.0700	0.0800
	0.0000	0.0101	0.0204	0.0309	0.0417	0.0526	0.0638	0.0753	0.0870
800.	(0.0000)	(-0.0005)	(-0.0022)	(-0.0050)	(-0.0091)	(-0.0145)	(-0.0213)	(-0.0296)	(-0.0395)
825.	(0.0000)	(-0.0005)	(-0.0022)	(-0.0050)	(-0.0091)	(-0.0145)	(-0.0214)	(-0.0297)	(-0.0397)
839.15	(0.0000)	(-0.0005)	(-0.0022)	(-0.0050)	(-0.0091)	(-0.0146)	(-0.0214)	(-0.0298)	(-0.0398)
850.	(0.0000)	(-0.0005)	(-0.0022)	(-0.0050)	(-0.0092)	(-0.0146)	(-0.0215)	(-0.0299)	(-0.0399)
875.	(0.0000)	(-0.0005)	(-0.0022)	(-0.0051)	(-0.0092)	(-0.0147)	(-0.0216)	(-0.0300)	-0.0401
900.	(0.0000)	(-0.0005)	(-0.0022)	(-0.0051)	(-0.0093)	(-0.0148)	(-0.0217)	(-0.0302)	-0.0403
925.	(0.0000)	(-0.0005)	(-0.0022)	(-0.0051)	(-0.0093)	(-0.0148)	(-0.0218)	-0.0303	-0.0405
950.	(0.0000)	(-0.0005)	(-0.0022)	(-0.0052)	(-0.0093)	(-0.0149)	(-0.0219)	-0.0305	-0.0407
1000.	(0.0000)	(-0.0006)	(-0.0023)	(-0.0052)	(-0.0094)	(-0.0151)	-0.0222	-0.0308	-0.0411
1050.	(0.0000)	(-0.0006)	(-0.0023)	(-0.0053)	(-0.0095)	(-0.0152)	-0.0224	-0.0311	-0.0415
1100.	(0.0000)	(-0.0006)	(-0.0023)	(-0.0053)	(-0.0096)	(-0.0154)	-0.0226	-0.0314	-0.0420
1150.	(0.0000)	(-0.0006)	(-0.0023)	(-0.0054)	(-0.0097)	-0.0155	-0.0228	-0.0317	-0.0424
1184.	(0.0000)	(-0.0006)	(-0.0023)	(-0.0054)	(-0.0098)	-0.0156	-0.0230	-0.0320	-0.0427
1184.	(0.0000)	(-0.0006)	(-0.0023)	(-0.0054)	(-0.0098)	-0.0156	-0.0230	-0.0320	-0.0427
1200.	(0.0000)	(-0.0006)	(-0.0024)	(-0.0054)	(-0.0098)	-0.0157	-0.0231	-0.0321	-0.0428
1250.	(0.0000)	(-0.0006)	(-0.0024)	(-0.0055)	(-0.0099)	-0.0158	-0.0233	-0.0324	-0.0432
1300.	(0.0000)	(-0.0006)	(-0.0024)	(-0.0055)	(-0.0100)	-0.0160	-0.0235	-0.0327	-0.0436
1350.	(0.0000)	(-0.0006)	(-0.0024)	(-0.0056)	(-0.0101)	-0.0161	-0.0237	-0.0330	-0.0440
1400.	(0.0000)	(-0.0006)	(-0.0024)	(-0.0056)	(-0.0102)	-0.0163	-0.0240	-0.0333	-0.0445
1450.	(0.0000)	(-0.0006)	(-0.0025)	(-0.0057)	(-0.0103)	-0.0164	-0.0242	-0.0336	-0.0449
1500.	(0.0000)	(-0.0006)	(-0.0025)	(-0.0057)	(-0.0104)	-0.0166	-0.0244	-0.0339	-0.0453
1550.	(0.0000)	(-0.0006)	(-0.0025)	(-0.0058)	(-0.0105)	-0.0167	-0.0246	-0.0342	-0.0457
1600.	(0.0000)	(-0.0006)	(-0.0025)	(-0.0058)	(-0.0106)	-0.0169	-0.0248	-0.0346	-0.0461
1645.	(0.0000)	(-0.0006)	(-0.0026)	(-0.0059)	(-0.0107)	-0.0170	-0.0251	-0.0348	-0.0465
1650.	(0.0000)	(-0.0006)	(-0.0026)	(-0.0059)	(-0.0107)	(-0.0170)	(-0.0251)	-0.0349	-0.0465
1665.	(0.0000)	(-0.0006)	(-0.0026)	(-0.0059)	(-0.0107)	(-0.0171)	(-0.0251)	(-0.0350)	(-0.0467)
1665.	(0.0000)	(-0.0006)	(-0.0026)	(-0.0059)	(-0.0107)	(-0.0171)	(-0.0251)	(-0.0350)	(-0.0467)
1697.15	(0.0000)	(-0.0006)	(-0.0026)	(-0.0059)	(-0.0108)	(-0.0172)	(-0.0253)	(-0.0352)	(-0.0469)
1700.	(0.0000)	(-0.0006)	(-0.0026)	(-0.0059)	(-0.0108)	(-0.0172)	(-0.0253)	(-0.0352)	(-0.0469)

Table 9.22 Continued. Activity of the FeO component, log a(FeO), in wustite, $Fe_{1-y}O$.

Temperature	Composition of Wustite: first line = "y", second line = "x" (moles)								
(K)	0.0800	0.0900	0.1000	0.1100	0.1200	0.1300	0.1400	0.1500	0.1600
	0.0870	0.0999	0.1111	0.1236	0.1364	0.1494	0.1628	0.1765	0.1905
800.	(-0.0395)	(-0.0511)	(-0.0644)	(-0.0797)	(-0.0971)	(-0.1165)	(-0.1383)	(-0.1625)	(-0.1894)
825.	(-0.0397)	(-0.0513)	(-0.0648)	(-0.0801)	(-0.0976)	(-0.1171)	(-0.1390)	(-0.1634)	(-0.1904)
839.15	(-0.0398)	(-0.0515)	(-0.0650)	(-0.0804)	(-0.0979)	(-0.1175)	(-0.1395)	(-0.1639)	(-0.1909)
850.	(-0.0399)	(-0.0516)	(-0.0651)	(-0.0806)	(-0.0981)	(-0.1178)	(-0.1398)	(-0.1643)	(-0.1914)
875.	-0.0401	(-0.0519)	(-0.0655)	(-0.0810)	(-0.0986)	(-0.1184)	(-0.1405)	(-0.1651)	(-0.1924)
900.	-0.0403	(-0.0521)	(-0.0658)	(-0.0814)	(-0.0991)	(-0.1190)	(-0.1412)	(-0.1660)	(-0.1934)
925.	-0.0405	-0.0524	(-0.0661)	(-0.0818)	(-0.0996)	(-0.1196)	(-0.1420)	(-0.1668)	(-0.1943)
950.	-0.0407	-0.0527	(-0.0665)	(-0.0822)	(-0.1001)	(-0.1202)	(-0.1427)	(-0.1677)	(-0.1953)
1000.	-0.0411	-0.0532	(-0.0672)	(-0.0831)	(-0.1011)	(-0.1214)	(-0.1441)	(-0.1694)	(-0.1973)
1050.	-0.0415	-0.0537	-0.0678	(-0.0839)	(-0.1022)	(-0.1227)	(-0.1456)	(-0.1711)	(-0.1993)
1100.	-0.0420	-0.0543	-0.0685	(-0.0848)	(-0.1032)	(-0.1239)	(-0.1471)	(-0.1728)	(-0.2013)
1150.	-0.0424	-0.0548	-0.0692	-0.0856	(-0.1042)	(-0.1251)	(-0.1485)	(-0.1745)	(-0.2033)
1184.	-0.0427	-0.0552	-0.0696	-0.0862	(-0.1049)	(-0.1260)	(-0.1495)	(-0.1757)	(-0.2047)
1184.	-0.0427	-0.0552	-0.0696	-0.0862	(-0.1049)	(-0.1260)	(-0.1495)	(-0.1757)	(-0.2047)
1200.	-0.0428	-0.0554	-0.0699	-0.0864	(-0.1052)	(-0.1264)	(-0.1500)	(-0.1762)	(-0.2053)
1250.	-0.0432	-0.0559	-0.0705	-0.0873	-0.1063	(-0.1276)	(-0.1514)	(-0.1779)	(-0.2073)
1300.	-0.0436	-0.0564	-0.0712	-0.0881	-0.1073	(-0.1288)	(-0.1529)	(-0.1797)	(-0.2093)
1350.	-0.0440	-0.0570	-0.0719	-0.0890	-0.1083	-0.1300	(-0.1543)	(-0.1814)	(-0.2113)
1400.	-0.0445	-0.0575	-0.0726	-0.0898	-0.1093	-0.1313	(-0.1558)	(-0.1831)	(-0.2133)
1450.	-0.0449	-0.0580	-0.0733	-0.0906	-0.1103	-0.1325	(-0.1573)	(-0.1848)	(-0.2153)
1500.	-0.0453	-0.0586	-0.0739	-0.0915	-0.1114	-0.1337	-0.1587	(-0.1865)	(-0.2173)
1550.	-0.0457	-0.0591	-0.0746	-0.0923	-0.1124	-0.1350	-0.1602	(-0.1882)	(-0.2193)
1600.	-0.0461	-0.0597	-0.0753	-0.0932	-0.1134	-0.1362	-0.1616	-0.1899	-0.2213
1645.	-0.0465	-0.0601	-0.0759	-0.0939	-0.1143	-0.1373	-0.1629	-0.1915	-0.2231
1650.	-0.0465	-0.0602	-0.0760	-0.0940	-0.1144	-0.1374	-0.1631	-0.1916	-0.2233
1665.	(-0.0467)	(-0.0604)	-0.0762	-0.0943	-0.1147	-0.1378	-0.1635	-0.1922	-0.2239
1665.	(-0.0467)	(-0.0604)	-0.0762	-0.0943	-0.1147	-0.1378	-0.1635	-0.1922	-0.2239
1697.15	(-0.0469)	(-0.0607)	(-0.0766)	(-0.0948)	(-0.1154)	(-0.1386)	(-0.1645)	(-0.1933)	(-0.2252)
1700.	(-0.0469)	(-0.0607)	(-0.0767)	(-0.0948)	(-0.1155)	(-0.1386)	(-0.1645)	(-0.1934)	(-0.2253)

Table 9.23 Thermodynamic properties of wustite (calorimetric sample), $Fe_{0.947}O(s)$, between 200 and 1700 K at a total pressure of one bar. This composition is metastable below about 1078 K relative to a more oxygen-rich wustite and metallic iron. It is also metastable above about 1650 K relative to an oxide liquid.

T	V°	S°	$\frac{-[G^\circ_T-H^\circ_{298}]}{T}$	$\frac{[H^\circ_T-H^\circ_{298}]}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log $_fK^\circ$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	12.038	39.088	-61.974	-22.886	46.353	-4577.	----	----	----
250.	12.040	49.266	-58.449	-9.183	46.545	-2296.	----	----	----
2 s	0.005	0.809	0.696	0.140	0.798	35.			
273.15	12.042	53.439	-57.850	-4.411	47.674	-1205.	----	----	----
298.15	12.046	57.659	-57.659	0.000	48.686	0.	-265518.	-244413.	42.819
2 s	0.004	0.705	0.705	0.000	0.674	0.	923.	713.	0.124
300.	12.046	57.960	-57.660	0.300	48.752	90.	----	----	----
350.	12.056	65.592	-58.259	7.333	50.207	2567.	----	----	----
400.	12.069	72.365	-59.607	12.758	51.197	5103.	----	----	----
450.	12.085	78.439	-61.368	17.071	51.918	7682.	----	----	----
500.	12.103	83.939	-63.354	20.585	52.480	10292.	----	----	----
2 s	0.007	0.425	0.641	0.256	0.649	128.			
550.	12.124	88.963	-65.457	23.506	52.946	12928.	----	----	----
600.	12.146	93.588	-67.611	25.977	53.351	15586.	----	----	----
650.	12.169	97.873	-69.776	28.097	53.721	18263.	----	----	----
700.	12.193	101.867	-71.928	29.939	54.069	20958.	----	----	----
750.	12.219	105.609	-74.050	31.559	54.404	23670.	----	----	----
2 s	0.007	0.214	0.522	0.367	0.621	275.			
800.	12.245	109.131	-76.134	32.997	54.733	26398.	-261733.	-211571.	13.814
825.	12.259	110.817	-77.158	33.659	54.896	27768.	-261701.	-210004.	13.296
839.15	12.266	111.752	-77.735	34.017	54.988	28546.	-261695.	-209117.	13.017
2 s	0.007	0.161	0.482	0.384	0.609	322.	673.	538.	0.033
------------------- Iron(alpha) - Wustite Solid Solution - Magnetite Coexistance -------------------									
850.	12.272	112.459	-78.173	34.286	55.059	29143.	-261696.	-208437.	12.809
875.	12.286	114.057	-79.176	34.881	55.222	30521.	-261720.	-206871.	12.349
900.	12.300	115.615	-80.166	35.449	55.386	31904.	-261780.	-205303.	11.915
925.	12.314	117.135	-81.145	35.990	55.550	33291.	-261880.	-203733.	11.504
950.	12.328	118.618	-82.111	36.507	55.714	34681.	-262029.	-202159.	11.115
1000.	12.357	121.484	-84.009	37.475	56.046	37475.	-262533.	-198997.	10.394
2 s	0.006	0.105	0.416	0.396	0.535	396.	638.	533.	0.027
1050.	12.386	124.227	-85.859	38.368	56.381	40286.	-263526.	-195797.	9.740
1100.	12.415	126.858	-87.664	39.194	56.721	43114.	-263938.	-192561.	9.144
1150.	12.444	129.387	-89.423	39.964	57.065	45958.	-264047.	-189313.	8.599
1184.	12.465	131.053	-90.595	40.458	57.302	47902.	-264043.	-187103.	8.254
- - - - - - - - - - - - - - - - - - -Fe(alpha) = Fe(gamma)- - - - - - - - - - - - - - - - - -									
1184.	12.465	131.053	-90.595	40.458	57.302	47902.	-264894.	-187103.	8.254
1200.	12.474	131.823	-91.140	40.683	57.414	48820.	-264776.	-186053.	8.098
1250.	12.504	134.173	-92.813	41.360	57.767	51700.	-264411.	-182780.	7.638
2 s	0.004	0.095	0.332	0.370	0.415	462.	652.	534.	0.022
1300.	12.534	136.446	-94.448	41.998	58.125	54597.	-264051.	-179522.	7.213
1350.	12.565	138.646	-96.044	42.602	58.487	57512.	-263697.	-176278.	6.820
1400.	12.595	140.780	-97.604	43.175	58.854	60446.	-263349.	-173047.	6.456
1450.	12.625	142.852	-99.130	43.722	59.225	63398.	-263005.	-169828.	6.118
1500.	12.656	144.866	-100.621	44.245	59.599	66368.	-262665.	-166620.	5.802
2 s	0.007	0.104	0.273	0.301	0.961	451.	695.	539.	0.018
1550.	12.687	146.826	-102.079	44.747	59.978	69358.	-262330.	-163424.	5.507
1600.	12.717	148.737	-103.508	45.229	60.361	72366.	-261998.	-160239.	5.231
1645.	12.745	150.416	-104.769	45.647	60.708	75090.	-261702.	-157381.	4.997
1650.	12.748	150.600	-104.907	45.693	60.747	75394.	-261669.	-157064.	4.972
1665.	12.757	151.150	-105.321	45.829	60.863	76306.	-261571.	-156114.	4.898
- - - - - - - - - - - - - - - - - - -Fe(gamma) = Fe(alpha)- - - - - - - - - - - - - - - - - -									
1665.	12.757	151.150	-105.321	45.829	60.863	76306.	-262363.	-156114.	4.898
1697.15	12.777	152.317	-106.201	46.116	61.114	78267.	-262253.	-154063.	4.742
1700.	12.779	152.419	-106.277	46.142	61.136	78441.	-262243.	-153882.	4.728
2 s	0.011	0.270	0.239	0.291	1.988	509.	1024.	552.	0.016

Table 9.24 Log a(Fe) and related properties in wustite (calorimetric sample), $Fe_{0.947}O$, between 800 and 1700 K at a total pressure of one bar. This composition is metastable below about 1078 K relative to a more oxygen-rich wustite and metallic iron. It is also metastable above about 1650 K relative to an oxide liquid.

Temperature	$\overline{S}(Fe)-\overline{S}^\circ(Fe)$	$\overline{H}(Fe)-\overline{H}^\circ(Fe)$	$\overline{G}(Fe)-\overline{G}^\circ(Fe)$	log a(Fe)
K	J/(mol·K)	------- J/mol	-------	
800.	38.915	38856.	7724.	0.504
825.	36.645	37012.	6780.	0.429
839.15	35.403	35978.	6270.	0.390
850.	34.470	35191.	5891.	0.362
875.	32.382	33390.	5056.	0.302
900.	30.373	31607.	4271.	0.248
925.	28.436	29840.	3536.	0.200
950.	26.564	28085.	2849.	0.157
1000.	22.996	24607.	1611.	0.084
1050.	19.635	21163.	546.	0.027
1100.	16.454	17744.	-356.	-0.017
1150.	13.430	14343.	-1102.	-0.050
1184.	11.456	12039.	-1525.	-0.067
1184.	9.726	9991.	-1525.	-0.067
1200.	8.970	9090.	-1674.	-0.073
1250.	6.665	6267.	-2065.	-0.086
1300.	4.438	3428.	-2342.	-0.094
1350.	2.280	568.	-2510.	-0.097
1400.	0.183	-2315.	-2571.	-0.096
1450.	-1.858	-5223.	-2529.	-0.091
1500.	-3.849	-8160.	-2386.	-0.083
1550.	-5.794	-11126.	-2145.	-0.072
1600.	-7.697	-14123.	-1808.	-0.059
1645.	-9.376	-16848.	-1423.	-0.045
1650.	-9.561	-17152.	-1376.	-0.044
1665.	-10.113	-18067.	-1229.	-0.039
1665.	-11.264	-19984.	-1229.	-0.039
1697.15	-12.508	-22074.	-847.	-0.026
1700.	-12.617	-22259.	-811.	-0.025

Table 9.25 Log $a(O_2)$ and related properties in wustite (calorimetric sample), $Fe_{0.947}O$, between 800 and 1700 K at a total pressure of one bar. This composition is metastable below about 1078 K relative to a more oxygen-rich wustite and metallic iron. It is also metastable above about 1650 K relative to an oxide liquid.

Temperature	$\overline{S}(O_2)-\overline{S}°(O_2)$	$\overline{H}(O_2)-\overline{H}°(O_2)$	$\overline{G}(O_2)-\overline{G}°(O_2)$	log $a(O_2)$
K	J/(mol·K)	------- J/mol -------		
800.	-197.608	-595823.	-437737.	-28.583
825.	-194.005	-592896.	-432842.	-27.405
839.15	-192.008	-591234.	-430111.	-26.772
850.	-190.497	-589958.	-428036.	-26.303
875.	-187.077	-587008.	-423316.	-25.270
900.	-183.741	-584048.	-418681.	-24.300
925.	-180.485	-581077.	-414128.	-23.387
950.	-177.303	-578094.	-409656.	-22.527
1000.	-171.149	-572095.	-400946.	-20.948
1050.	-165.253	-566052.	-392537.	-19.532
1100.	-159.589	-559965.	-384417.	-18.256
1150.	-154.138	-553833.	-376575.	-17.102
1184.	-150.543	-549638.	-371395.	-16.381
1184.	-150.543	-549638.	-371395.	-16.381
1200.	-148.881	-547656.	-369000.	-16.059
1250.	-143.802	-541436.	-361684.	-15.112
1300.	-138.887	-535170.	-354617.	-14.248
1350.	-134.124	-528860.	-347792.	-13.457
1400.	-129.503	-522506.	-341202.	-12.731
1450.	-125.012	-516107.	-334840.	-12.063
1500.	-120.643	-509664.	-328699.	-11.447
1550.	-116.389	-503176.	-322774.	-10.878
1600.	-112.241	-496644.	-317058.	-10.351
1645.	-108.594	-490727.	-312090.	-9.909
1650.	-108.194	-490067.	-311548.	-9.862
1665.	-106.998	-488086.	-309934.	-9.722
1665.	-106.998	-488086.	-309934.	-9.722
1697.15	-104.463	-483825.	-306535.	-9.434
1700.	-104.240	-483446.	-306237.	-9.409

Table 9.26 Log a(FeO) and related properties in wustite (calorimetric sample), $Fe_{0.947}O$, between 800 and 1700 K at a total pressure of one bar. This composition is metastable below about 1078 K relative to a more oxygen-rich wustite and metallic iron. It is also metastable above about 1650 K relative to an oxide liquid.

Temperature	$\overline{S}$(FeO)-$\overline{S}^\circ$(FeO)	$\overline{H}$(FeO)-$\overline{H}^\circ$(FeO)	$\overline{G}$(FeO)-$\overline{G}^\circ$(FeO)	log a(FeO)
K	J/(mol·K)	J/mol		
800.	0.366	42.	-250.	-0.016
825.	0.369	45.	-260.	-0.016
839.15	0.371	46.	-265.	-0.016
850.	0.372	48.	-269.	-0.017
875.	0.376	50.	-278.	-0.017
900.	0.379	53.	-288.	-0.017
925.	0.382	56.	-297.	-0.017
950.	0.386	60.	-307.	-0.017
1000.	0.392	66.	-326.	-0.017
1050.	0.399	73.	-346.	-0.017
1100.	0.405	80.	-366.	-0.017
1150.	0.412	87.	-386.	-0.018
1184.	0.416	92.	-401.	-0.018
1184.	0.416	92.	-401.	-0.018
1200.	0.418	95.	-407.	-0.018
1250.	0.425	103.	-428.	-0.018
1300.	0.432	111.	-450.	-0.018
1350.	0.438	120.	-471.	-0.018
1400.	0.445	129.	-494.	-0.018
1450.	0.451	139.	-516.	-0.019
1500.	0.458	148.	-539.	-0.019
1550.	0.465	158.	-562.	-0.019
1600.	0.471	169.	-585.	-0.019
1645.	0.477	178.	-607.	-0.019
1650.	0.478	180.	-609.	-0.019
1665.	0.480	183.	-616.	-0.019
1665.	0.480	183.	-616.	-0.019
1697.15	0.484	190.	-632.	-0.019
1700.	0.484	191.	-633.	-0.019

Table 10.1. Recommended thermodynamic data at one bar total pressure for the reaction:

$2\ Cu_2O(\text{cuprite}) = 4\ Cu(\text{copper}) + O_2(g)$

The string "----" indicates that the property was not evaluated in this study.

T K	$\Delta_r H°$ J/mol	$\Delta_r G°$ J/mol	log $f(O_2)$	$_r E°$ volts	$\Delta_r V°$(solids) cm^3/mol
200.	340597.	310572.	-81.111	-0.8047	----
250.	341062.	303006.	-63.308	-0.7851	----
2 s	442.	434.	0.091	0.0011	----
273.15	341184.	299477.	-57.268	-0.7760	----
298.15	341262.	295655.	-51.797	-0.7661	----
2 s	453.	432.	0.076	0.0011	----
300.	341266.	295372.	-51.428	-0.7653	----
350.	341279.	287720.	-42.939	-0.7455	----
400.	341150.	280076.	-36.573	-0.7257	----
450.	340912.	272455.	-31.625	-0.7060	----
500.	340585.	264866.	-27.670	-0.6863	----
2 s	559.	396.	0.041	0.0010	----
550.	340186.	257313.	-24.437	-0.6667	----
600.	339725.	249799.	-21.746	-0.6472	----
650.	339213.	242325.	-19.473	-0.6279	----
700.	338659.	234893.	-17.528	-0.6086	----
750.	338070.	227501.	-15.844	-0.5895	----
2 s	683.	307.	0.021	0.0008	----
800.	337454.	220150.	-14.374	-0.5704	----
850.	336818.	212838.	-13.079	-0.5515	----
900.	336168.	205564.	-11.930	-0.5326	----
950.	335510.	198326.	-10.904	-0.5139	----
1000.	334850.	191123.	-9.983	-0.4952	----
2 s	734.	225.	0.012	0.0006	----
1050.	334194.	183953.	-9.151	-0.4766	----
1100.	333545.	176814.	-8.396	-0.4581	----
1150.	332910.	169704.	-7.708	-0.4397	----
1200.	332293.	162621.	-7.079	-0.4214	----
1250.	331698.	155564.	-6.501	-0.4031	----
2 s	1019.	215.	0.009	0.0006	----
1300.	331130.	148530.	-5.968	-0.3849	----
1350.	330591.	141517.	-5.476	-0.3667	----
1357.6	330512.	140453.	-5.404	-0.3639	----
2 s	1314.	264.	0.010	0.0007	----

Table 10.2. Recommended thermodynamic data at one bar total pressure for the reaction:

$4\ CuO(tenorite) = 2\ Cu_2O(cuprite) + O_2(g)$

The string "----" indicates that the property was not evaluated in this study.

T K	$\Delta_r H°$ J/mol	$\Delta_r G°$ J/mol	log $f(O_2)$	$_r E°$ volts	$\Delta_r V°$(solids) cm^3/mol
200.	282431.	237688.	-62.077	-0.6159	----
227.	282176.	231661.	-53.306	-0.6002	----
T_N (CuO)					
227.	282176.	231661.	-53.306	-0.6002	----
250.	281942.	226555.	-47.335	-0.5870	----
2 s	863.	838.	0.175	0.0022	----
273.15	281700.	221436.	-42.345	-0.5738	----
298.15	281377.	215935.	-37.830	-0.5595	----
2 s	884.	832.	0.146	0.0022	----
300.	281350.	215529.	-37.526	-0.5584	----
350.	280517.	204621.	-30.537	-0.5302	----
400.	279508.	193846.	-25.313	-0.5023	----
450.	278387.	183205.	-21.265	-0.4747	----
500.	277200.	172692.	-18.041	-0.4475	----
2 s	1110.	755.	0.079	0.0020	----
550.	275980.	162300.	-15.414	-0.4205	----
600.	274746.	152020.	-13.234	-0.3939	----
650.	273512.	141843.	-11.398	-0.3675	----
700.	272287.	131761.	-9.832	-0.3414	----
750.	271075.	121765.	-8.480	-0.3155	----
2 s	1368.	555.	0.039	0.0014	----
800.	269879.	111850.	-7.303	-0.2898	----
850.	268701.	102010.	-6.269	-0.2643	----
900.	267540.	92238.	-5.353	-0.2390	----
950.	266396.	82530.	-4.538	-0.2138	----
1000.	265267.	72882.	-3.807	-0.1888	----
2 s	1481.	332.	0.017	0.0009	----
1050.	264151.	63291.	-3.148	-0.1640	----
1100.	263048.	53752.	-2.552	-0.1393	----
1150.	261954.	44263.	-2.010	-0.1147	----
1200.	260868.	34821.	-1.516	-0.0902	----
1250.	259787.	25425.	-1.062	-0.0659	----
2 s	1584.	301.	0.013	0.0008	----
1300.	258710.	16072.	-0.646	-0.0416	----
1350.	257635.	6760.	-0.262	-0.0175	----
1400.	256559.	-2512.	0.094	0.0065	----
1450.	255480.	-11746.	0.423	0.0304	----
1500.	254397.	-20942.	0.729	0.0543	----
2 s	3359.	599.	0.021	0.0016	----
1516.7	254034.	-24005.	0.827	0.0622	----
2 s	3568.	634.	0.022	0.0016	----

Table 10.3. Recommended thermodynamic data at one bar total pressure for the reaction:

$2\ NiO(bunsenite) = 2\ Ni(nickel) + O_2(g)$

Refer to the text for a discussion of the use of $\Delta_r V°$(solids).

T K	$\Delta_r H°$ J/mol	$\Delta_r G°$ J/mol	log $f(O_2)$	$_r E°$ volts	$\Delta_r V°$(solids) cm^3/mol
200.	480600.	442270.	-115.507	-1.1460	-8.8313
250.	480748.	432664.	-90.398	-1.1211	-8.8465
2 s	749.	587.	0.123	0.0015	0.0308
273.15	480699.	428213.	-81.886	-1.1095	-8.8535
298.15	480555.	423415.	-74.179	-1.0971	-8.8610
2 s	747.	557.	0.098	0.0014	0.0309
300.	480541.	423061.	-73.660	-1.0962	-8.8616
350.	479984.	413520.	-61.713	-1.0715	-8.8767
400.	479127.	404081.	-52.766	-1.0470	-8.8917
450.	477987.	394765.	-45.822	-1.0229	-8.9068
500.	476474.	385595.	-40.282	-0.9991	-8.9218
2 s	752.	430.	0.045	0.0011	0.0312
519.	475709.	382155.	-38.461	-0.9902	-8.9275
		T_N (NiO)			
519.	475709.	382155.	-38.461	-0.9902	-8.9275
550.	474909.	376594.	-35.765	-0.9758	-8.9368
600.	474253.	367689.	-32.009	-0.9527	-8.9518
631.	474105.	362188.	-29.982	-0.9385	-8.9611
		T_N (Ni)			
631.	474105.	362188.	-29.981	-0.9385	-8.9611
650.	473918.	358821.	-28.835	-0.9297	-8.9668
700.	473258.	349991.	-26.116	-0.9069	-8.9818
750.	472535.	341211.	-23.764	-0.8841	-8.9967
2 s	740.	280.	0.020	0.0007	0.0309
800.	471796.	332480.	-21.708	-0.8615	-9.0117
850.	471059.	323796.	-19.898	-0.8390	-9.0267
900.	470335.	315154.	-18.291	-0.8166	-9.0416
950.	469630.	306552.	-16.855	-0.7943	-9.0566
1000.	468946.	297987.	-15.565	-0.7721	-9.0715
2 s	705.	159.	0.008	0.0004	0.0318
1050.	468284.	289455.	-14.399	-0.7500	-9.0865
1100.	467646.	280955.	-13.341	-0.7280	-9.1014
1150.	467029.	272483.	-12.376	-0.7060	-9.1163
1200.	466434.	264037.	-11.493	-0.6841	-9.1313
1250.	465858.	255616.	-10.681	-0.6623	-9.1462
2 s	717.	125.	0.005	0.0003	0.0353
1300.	465300.	247217.	-9.933	-0.6406	-9.1611
1350.	464757.	238840.	-9.241	-0.6188	-9.1761
1400.	464229.	230482.	-8.599	-0.5972	-9.1910
1450.	463712.	222143.	-8.002	-0.5756	-9.2059
1500.	463204.	213822.	-7.446	-0.5540	-9.2209
2 s	860.	225.	0.008	0.0006	0.0412
1550.	462704.	205517.	-6.926	-0.5325	-9.2358
1600.	462209.	197229.	-6.439	-0.5110	-9.2507
1650.	461718.	188956.	-5.982	-0.4896	-9.2657
1700.	461228.	180698.	-5.552	-0.4682	-9.2806
1728.	460953.	176079.	-5.322	-0.4562	-9.2890
2 s	1200.	376.	0.011	0.0010	0.0480

Table 10.4. Recommended thermodynamic data at one bar total pressure for the reaction:

$$2\ Fe_{1-y}O(\text{wustite}) = 2(1-y)\ Fe(\text{iron}) + O_2(g)$$

The string "----" indicates that the property was not calculated in this study. The composition of the wustite solid solution is varying along the buffer curve. These details are given in Chapter 9 on Table 9.01. The effect of pressure on the location of the buffer curve is complex because the composition of wustite varies with pressure and temperature.

T K	y moles	x moles	$\Delta_r H°$ J/mol	$\Delta_r G°$ J/mol	log f(O2)	${}_rE°$ volts	$\Delta_r V°$(solids) cm^3/mol
839.15	0.0830	0.0905	525572.	418426.	-26.045	-1.0842	-10.9997
850.	0.0809	0.0880	525378.	417042.	-25.628	-1.0806	-10.9880
900.	0.0722	0.0778	524798.	410688.	-23.835	-1.0641	-10.9429
950.	0.0651	0.0697	524756.	404352.	-22.232	-1.0477	-10.9107
1000.	0.0595	0.0633	525392.	398004.	-20.789	-1.0313	-10.8895
1050.	0.0551	0.0583	527138.	391596.	-19.480	-1.0147	-10.8776
1100.	0.0517	0.0545	527832.	385122.	-18.287	-0.9979	-10.8738
1150.	0.0492	0.0517	527992.	378630.	-17.197	-0.9811	-10.8768
1184.	0.0479	0.0503	527970.	374214.	-16.509	-0.9696	-10.8822
T_t (Fe, α=γ)							
1184.	0.0479	0.0503	527970.	374214.	-16.509	-0.9696	-10.8822
1200.	0.0475	0.0499	527940.	372136.	-16.198	-0.9642	-10.8863
1250.	0.0465	0.0488	527768.	365648.	-15.279	-0.9474	-10.9017
1300.	0.0460	0.0482	527516.	359168.	-14.431	-0.9306	-10.9207
1350.	0.0458	0.0480	527210.	352698.	-13.646	-0.9139	-10.9427
1400.	0.0460	0.0482	526868.	346242.	-12.918	-0.8971	-10.9673
1450.	0.0464	0.0487	526500.	339796.	-12.240	-0.8804	-10.9942
1500.	0.0471	0.0494	526118.	333366.	-11.609	-0.8638	-11.0230
1550.	0.0479	0.0503	525728.	326946.	-11.018	-0.8471	-11.0535
1600.	0.0489	0.0514	525336.	320540.	-10.464	-0.8305	-11.0854
1650.	0.0500	0.0526	524946.	314146.	-9.945	-0.8140	-11.1185
1665.	0.0503	0.0530	524830.	312230.	-9.795	-0.8090	-11.1286
T_t (Fe, γ=α)							
1665.	0.0503	0.0530	524830.	312230.	-9.795	-0.8090	-11.1286
1700.	0.0513	0.0541	524560.	307764.	-9.456	-0.7974	-11.1533
1750.	0.0527	0.0557	524184.	301394.	-8.996	-0.7809	-11.1893
1800.	0.0542	0.0574	523820.	295034.	-8.561	-0.7645	-11.2261

Table 10.5. Recommended thermodynamic data at one bar total pressure for the reaction:

0.5 Fe_3O_4(magnetite) = 1.5 Fe(iron) + O_2(g)

Refer to the text for a discussion of the use of Δ_rV°(solids).

T K	Δ_rH° J/mol	Δ_rG° J/mol	log f(O_2)	$_rE^\circ$ volts	Δ_rV°(solids) cm^3/mol
200.	558614.	523724.	-136.780	-1.3570	-11.6250
250.	558605.	514996.	-107.600	-1.3344	-11.6288
2 s	1121.	1081.	0.283	0.0056	0.0063
273.15	558499.	510962.	-97.710	-1.3239	-11.6324
298.15	558320.	506619.	-88.756	-1.3127	-11.6375
2 s	1123.	1075.	0.189	0.0055	0.0068
300.	558304.	506298.	-88.152	-1.3119	-11.6379
350.	557773.	497669.	-74.272	-1.2895	-11.6517
400.	557067.	489129.	-63.872	-1.2674	-11.6693
450.	556228.	480686.	-55.795	-1.2455	-11.6903
500.	555281.	472343.	-49.344	-1.2239	-11.7140
2 s	1123.	1048.	0.110	0.0054	0.0080
550.	554239.	464099.	-44.075	-1.2025	-11.7402
600.	553103.	455953.	-39.693	-1.1814	-11.7683
650.	551865.	447907.	-35.993	-1.1606	-11.7981
700.	550499.	439961.	-32.830	-1.1400	-11.8293
750.	548950.	432118.	-30.095	-1.1196	-11.8618
2 s	1120.	1012.	0.071	0.0052	0.0066
800.	547090.	424387.	-27.709	-1.0996	-11.8952
839.15	545167.	418426.	-26.045	-1.0842	-11.9221
2 s	1122.	1000.	0.062	0.0051	0.0064

Table 10.6. Recommended thermodynamic data at one bar total pressure for the reaction:

Fe_2SiO_4(fayalite) = 2 Fe(iron) + SiO_2(quartz) + O_2(g)

Refer to the text for a discussion of the use of $\Delta_r V°$(solids).

T K	$\Delta_r H°$ J/mol	$\Delta_r G°$ J/mol	log $f(O_2)$	$_r E°$ volts	$\Delta_r V°$(solids) cm^3/mol
200.	567326.	537058.	-140.262	-1.3916	-9.3008
250.	567312.	529486.	-110.628	-1.3719	-9.2977
2 s	1324.	1116.	0.233	0.0029	0.0245
273.15	567205.	525988.	-100.583	-1.3629	-9.2946
298.15	567031.	522223.	-91.489	-1.3531	-9.2903
2 s	1324.	1078.	0.189	0.0028	0.0244
300.	567016.	521945.	-90.877	-1.3524	-9.2900
350.	566533.	514469.	-76.779	-1.3330	-9.2784
400.	565940.	507071.	-66.215	-1.3139	-9.2635
450.	565295.	499751.	-58.008	-1.2949	-9.2458
500.	564643.	492503.	-51.450	-1.2761	-9.2258
2 s	1340.	927.	0.097	0.0024	0.0244
550.	564017.	485320.	-46.091	-1.2575	-9.2038
600.	563449.	478191.	-41.629	-1.2390	-9.1800
650.	562966.	471107.	-37.858	-1.2207	-9.1549
700.	562598.	464055.	-34.628	-1.2024	-9.1285
750.	562376.	457025.	-31.829	-1.1842	-9.1011
2 s	1416.	751.	0.052	0.0019	0.0243
800.	562333.	450004.	-29.382	-1.1660	-9.0728
845.5	562486.	443612.	-27.406	-1.1494	-9.0465
			$T_t(SiO_2, \alpha = \beta)$		
845.5	563375.	443612.	-27.406	-1.1494	-8.7507
850.	563378.	442975.	-27.221	-1.1478	-8.7532
900.	563543.	435889.	-25.298	-1.1294	-8.7820
950.	564021.	428786.	-23.576	-1.1110	-8.8133
1000.	565019.	421645.	-22.024	-1.0925	-8.8466
2 s	1527.	616.	0.032	0.0016	0.0242
1050.	567041.	414431.	-20.616	-1.0738	-8.8817
1100.	567841.	407141.	-19.333	-1.0549	-8.9183
1150.	568012.	399831.	-18.161	-1.0360	-8.9561
1184.	567974.	394859.	-17.420	-1.0231	-8.9825
			T_t (Fe, $\alpha = \gamma$)		
1184.	569773.	394859.	-17.420	-1.0231	-9.1794
1200.	569514.	392497.	-17.085	-1.0170	-9.1880
1250.	568731.	385138.	-16.094	-0.9979	-9.2155
2 s	1743.	606.	0.025	0.0016	0.0248
1300.	567994.	377809.	-15.180	-0.9789	-9.2436
1350.	567306.	370507.	-14.335	-0.9600	-9.2721
1400.	566673.	363230.	-13.552	-0.9412	-9.3010
1450.	566096.	355974.	-12.823	-0.9224	-9.3302
1500.	565579.	348738.	-12.144	-0.9036	-9.3598
2 s	2531.	799.	0.028	0.0021	0.0253
1550.	565123.	341518.	-11.509	-0.8849	-9.3895
1600.	564732.	334311.	-10.914	-0.8662	-9.4195
1650.	564407.	327115.	-10.355	-0.8476	-9.4496
1665.	564322.	324959.	-10.194	-0.8420	-9.4586
			T_t (Fe, $\gamma = \alpha$)		
1665.	565995.	324959.	-10.194	-0.8420	-9.3856
1700.	566049.	319891.	-9.829	-0.8289	-9.4162
1750.	566209.	312649.	-9.332	-0.8101	-9.4600
2 s	4347.	1259.	0.038	0.0033	0.0268
1800.	566472.	305401.	-8.862	-0.7913	-9.5039
2 s	4844.	1390.	0.040	0.0036	0.0271

Table 10.7. Recommended thermodynamic data at one bar total pressure for the reaction:

$$(2-2y)/(1-4y)\ Fe_3O_4(\text{magnetite}) = 6/(1-4y)\ Fe_{1-y}O(\text{wustite}) + O_2(g)$$

The string "----" indicates that the property was not calculated in this study. The composition of the wustite solid solution is varying along the buffer curve. These details are given in Chapter 9 on Table 9.02. The effect of pressure on the location of the buffer curve is complex because the composition of wustite varies with pressure and temperature.

T K	y moles	x moles	$\Delta_r H°$ J/mol	$\Delta_r G°$ J/mol	log f(02)	$_rE°$ volts	$\Delta_r V°$(solids) cm^3/mol
839.15	0.0830	0.0905	633166.	418426.	-26.045	-1.0842	-16.0646
850.	0.0842	0.0919	629869.	415670.	-25.543	-1.0770	-16.0753
900.	0.0893	0.0980	624602.	403253.	-23.404	-1.0449	-16.1257
950.	0.0942	0.1040	623224.	391015.	-21.499	-1.0131	-16.1775
1000.	0.0989	0.1098	623286.	378795.	-19.786	-0.9815	-16.2304
1050.	0.1035	0.1155	624173.	366563.	-18.235	-0.9498	-16.2839
1100.	0.1080	0.1211	625707.	354265.	-16.822	-0.9179	-16.3375
1150.	0 1125	0.1268	627809.	341900.	-15.529	-0.8859	-16.3906
1200.	0.1170	0.1324	630491.	329411.	-14.339	-0.8535	-16.4429
1250.	0.1214	0.1382	633788.	316814.	-13.239	-0.8209	-16.4941
1300.	0.1259	0.1440	637741.	304064.	-12.217	-0.7879	-16.5436
1350.	0.1304	0.1499	642435.	291137.	-11.264	-0.7544	-16.5912
1400.	0.1349	0.1560	647976.	278026.	-10.373	-0.7204	-16.6366
1450.	0.1395	0.1622	654428.	264702.	-9.535	-0.6859	-16.6790
1500.	0.1442	0.1685	661916.	251132.	-8.745	-0.6507	-16.7181
1550.	0.1489	0.1749	670624.	237295.	-7.997	-0.6148	-16.7534
1600.	0.1536	0.1815	680681.	223152.	-7.285	-0.5782	-16.7842
1650.	0.1584	0.1883	692324.	208676.	-6.606	-0.5407	-16.8096
1700.	0.1633	0.1952	705777.	193826.	-5.955	-0.5022	-16.8299
1750.	0 1682	0.2022	721413.	178550.	-5.329	-0.4626	-16.8409
1800.	0.1731	0.2094	739582.	162798.	-4.724	-0.4218	-16.3443

Table 10.8. Recommended thermodynamic data at one bar total pressure for the reaction:

$$2\ Fe_3O_4(\text{magnetite}) + 3\ SiO_2(\text{quartz}) = 3\ Fe_2SiO_4(\text{fayalite}) + O_2(g)$$

Refer to the text for a discussion of the use of $\Delta_rV°$(solids).

T K	$\Delta_rH°$ J/mol	$\Delta_rG°$ J/mol	log f(O_2)	$_rE°$ volts	$\Delta_rV°$(solids) cm^3/mol
200.	532477.	483721.	-126.332	-1.2534	-18.5978
250.	532484.	471525.	-98.518	-1.2218	-18.6220
2 s	4007.	3368.	0.704	0.0087	0.0757
273.15	532381.	465884.	-89.089	-1.2071	-18.6456
298.15	532187.	459806.	-80.554	-1.1914	-18.6790
2 s	4005.	3253.	0.570	0.0084	0.0764
300.	532169.	459357.	-79.979	-1.1902	-18.6817
350.	531494.	447270.	-66.750	-1.1589	-18.7716
400.	530450.	435304.	-56.844	-1.1279	-18.8869
450.	529026.	423493.	-49.157	-1.0973	-19.0237
500.	527194.	411861.	-43.026	-1.0672	-19.1788
2 s	4055.	2792.	0.292	0.0072	0.0786
550.	524903.	400434.	-38.029	-1.0376	-19.3494
600.	522067.	389240.	-33.886	-1.0085	-19.5330
650.	518562.	378308.	-30.401	-0.9802	-19.7277
700.	514200.	367676.	-27.436	-0.9527	-19.9318
750.	508673.	357395.	-24.891	-0.9260	-20.1438
2 s	4285.	2254.	0.157	0.0058	0.0765
800.	501363.	347535.	-22.691	-0.9005	-20.3625
845.5	491650.	339037.	-20.945	-0.8785	-20.5665
T_t(SiO_2, α=β)					
845.5	488985.	339037.	-20.945	-0.8785	-21.4537
849.1	488033.	338400.	-20.817	-0.8768	-21.4578
T_N (Fe_3O_4)					
849.1	488033.	338400.	-20.817	-0.8768	-21.4578
850.	487850.	338242.	-20.785	-0.8764	-21.4588
900.	482742.	329617.	-19.130	-0.8541	-21.5126
950.	480451.	321178.	-17.659	-0.8322	-21.5616
1000.	479038.	312834.	-16.340	-0.8106	-21.6065
2 s	4607.	1846.	0.096	0.0048	0.0786
1050.	478020.	304550.	-15.150	-0.7891	-21.6480
1100.	477187.	296310.	-14.070	-0.7678	-21.6865
1150.	476440.	288105.	-13.086	-0.7465	-21.7226
1200.	475719.	279932.	-12.185	-0.7253	-21.7565
1250.	474990.	271789.	-11.357	-0.7042	-21.7887
2 s	5249.	1819.	0.076	0.0047	0.0917
1300.	474226.	263676.	-10.594	-0.6832	-21.8193
1350.	473406.	255593.	-9.889	-0.6623	-21.8487
1400.	472514.	247542.	-9.236	-0.6414	-21.8770
1450.	471534.	239525.	-8.628	-0.6206	-21.9044
1500.	470454.	231542.	-8.063	-0.5999	-21.9310
2 s	7649.	2405.	0.084	0.0062	0.1144
1550.	469259.	223598.	-7.535	-0.5794	-21.9570
1600.	467940.	215694.	-7.042	-0.5589	-21.9824
1650.	466485.	207834.	-6.579	-0.5385	-22.0074
1700.	464885.	200019.	-6.146	-0.5183	-22.0319
1750.	463130.	192254.	-5.738	-0.4981	-22.0562
	13143.	3796.	0.113	0.0098	0.1429
1800.	461211.	184542.	-5.355	-0.4782	-22.0801
	14645.	4193.	0.122	0.0109	0.1490

Table 10.9. Recommended thermodynamic data at one bar total pressure for the reaction:

$$6\ Fe_2O_3(\text{hematite}) = 4\ Fe_3O_4(\text{magnetite}) + O_2(g)$$

Refer to the text for a discussion of the use of Δ_rV°(solids).

T K	Δ_rH° J/mol	Δ_rG° J/mol	log $f(O_2)$	${}_rE^\circ$ volts	Δ_rV°(solids) cm^3/mol
200.	481096.	430344.	-112.392	-1.1150	-3.4843
250.	482479.	417473.	-87.224	-1.0817	-3.4971
2 s	1400.	1182.	0.247	0.0031	0.1207
273.15	482804.	411437.	-78.678	-1.0661	-3.4937
298.15	483013.	404895.	-70.935	-1.0491	-3.4842
2 s	1410.	1145.	0.201	0.0030	0.0989
300.	483024.	404411.	-70.413	-1.0479	-3.4833
350.	483180.	391293.	-58.396	-1.0139	-3.4469
400.	483229.	378163.	-49.382	-0.9798	-3.3914
450.	483341.	365024.	-42.370	-0.9458	-3.3197
500.	483637.	351864.	-36.758	-0.9117	-3.2344
2 s	1541.	972.	0.102	0.0025	0.0978
550.	484232.	338661.	-32.163	-0.8775	-3.1375
600.	485265.	325386.	-28.327	-0.8431	-3.0308
650.	486924.	312001.	-25.072	-0.8084	-2.9158
700.	489489.	298456.	-22.271	-0.7733	-2.7938
750.	493436.	284683.	-19.827	-0.7376	-2.6659
2 s	1706.	692.	0.048	0.0018	0.0839
800.	499795.	270577.	-17.667	-0.7011	-2.5329
849.1	511684.	256199.	-15.760	-0.6638	-2.3981
		T_N (Fe_3O_4)			
849.1	511684.	256199.	-15.760	-0.6638	-2.3981
850.	511886.	255928.	-15.727	-0.6631	-2.3956
900.	512022.	240800.	-13.975	-0.6239	-2.2548
950.	503240.	225938.	-12.423	-0.5854	-2.1109
955.53	501782.	224328.	-12.263	-0.5812	-2.0948
		T_N (Fe_2O_3)			
955.53	501782.	224328.	-12.263	-0.5812	-2.0948
1000.	497950.	211522.	-11.049	-0.5481	-1.9644
2 s	1678.	419.	0.022	0.0011	0.0809
1050.	496220.	197248.	-9.812	-0.5111	-1.8157
1100.	495196.	183037.	-8.692	-0.4743	-1.6652
1150.	494446.	168865.	-7.670	-0.4375	-1.5131
1200.	493803.	154724.	-6.735	-0.4009	-1.3597
1250.	493191.	140608.	-5.876	-0.3643	-1.2051
2 s	1306.	263.	0.011	0.0007	0.1555
1300.	492575.	126517.	-5.083	-0.3278	-1.0496
1350.	491941.	112450.	-4.351	-0.2914	-0.8933
1400.	491281.	98406.	-3.672	-0.2550	-0.7364
1450.	490596.	84387.	-3.040	-0.2187	-0.5788
1500.	489886.	70392.	-2.451	-0.1824	-0.4208
2 s	1969.	208.	0.007	0.0005	0.2611
1550.	489153.	56421.	-1.901	-0.1462	-0.2623
1600.	488402.	42474.	-1.387	-0.1101	-0.1035
1650.	487636.	28550.	-0.904	-0.0740	0.0556
1700.	486859.	14650.	-0.450	-0.0380	0.2150
1750.	486075.	773.	-0.023	-0.0020	0.3745
2 s	3914.	533.	0.016	0.0014	0.3762
1800.	485289.	-13082.	0.380	0.0339	0.5343
2 s	4401.	653.	0.019	0.0017	0.3998

Table A.01. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$2\ Cu(s) + 0.5\ O_2(g) = Cu_2O(cuprite)$

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-170.631±0.226
Average of flagged studies below.			-170.689
* Mah and others(1967)	298.15	1	-170.832±1.250
* Fischer and Pateisky (1970)	873-1356	eqn	-170.394±0.124
* Holmes and others (1986)	891-1341	29	-170.438±0.108
* Kemori and others (1979)	1183-1332	16	-170.940±0.034
Kodera and others (1968)	1200-1425	eqn	-169.700±1.621
Matsushita and Goto (1963)	773-1323	eqn	-172.232±0.317
Peters (1983)	973-1323	eqn	-174.775±0.074
* Rizzo and others (1967)	973-1273	eqn	-170.298±0.116
* Slobodyanyuk and others (1973)	1073-1273	eqn	-171.138±0.050
Treadwell (1916)	1173-1273	5	-164.586±0.698
* Tretyakov and Schmalzreid (1965)	1000-1500	eqn	-170.784±0.348

Table A.02. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

Cu_2O(cuprite) + CO(g) = 2 Cu(s) + CO_2(g)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-112.350±0.226
Peters and Mann (1958)	1073-1273	eqn	-115.156±0.261

Table A.03. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

2 Cu(s) + O_2(g) = 2 CuO(tenorite)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-311.320±0.418
Average of flagged studies below.			-311.540
* Mah and others (1967)	298.15	1	-311.540±0.625
Matsushita and Goto (1963)	773-1323	eqn	-317.446±3.803

Table A.04. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

Cu_2O(cuprite) + 0.5 O_2 = 2 CuO(tenorite)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-140.688±0.442
Average of flagged studies below.			-140.779
* Hochgeschwender and Ingraham (1967)	1022-1294	46	-140.561±0.280
Kodera and others (1968)	875-1175	eqn	-146.536±0.262
* Landolt and Muan (1969)	1223-1323	6	-140.949±0.068
Norton (1955)	773-1273	eqn	-140.100±0.879
Peters (1983)	973-1323	eqn	-143.101±1.238
* Rog (1976)	873-1273	eqn	-140.607±0.131
* Slobodyanyuk and others (1973)	973-1123	5	-141.054±0.750
Treadwell (1916)	1213-1273	6	-137.402±3.230
* Vasileva and others (1975)	1073-1273	9	-140.726±0.166

Table A.05. Comparison of the third-law $\Delta_r H^\circ(298)$ from all studies with the results of this study for the reaction:

$Ni(s) + 0.5\ O_2(g) = NiO(bunsenite)$

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H^\circ(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-240.277±0.374
Average of flagged studies below.			-239.939
* Boyle and others (1954)	298.15	1	-239.734±0.418
Barbi (1964a)	850-1283	eqn	-239.881±0.676
	842-1273	eqn	-239.286±1.767
Berglund (1976)	850-1650	17	-239.529±0.456
* Charette (1967)	911-1376	13	-239.956±0.126
Commert and Pratt (1984)	760-1275	eqn	-240.164±0.340
* Fischer and Pateisky (1970)	873-1723	eqn	-239.986±0.474
* Grimley and others (1961)	1575-1709	19	-239.107±1.184
* Holmes and others(1986)	890-1439	42	-240.434±0.218
Huebner and Sato (1970)			
Run 1	792-1594	30	-240.754±2.228
Run 2	846-1488	16	-241.948±0.694
Run 3	818-1474	45	-238.958±2.760
Run 4	985-1458	27	-236.806±2.862
* Iwase and others (1975,1978)	973-1673	eqn	-239.406±0.224
Kazenas and others (1969)	1400-1580	eqn	-235.181±0.023
* Kemori and others (1979)	1191-1722	46	-240.108±0.290
* Kodera and others (1968)	1400-1575	eqn	-239.852±0.129
* Meier and Rapp (1971)	973-1473	eqn	-240.188±1.783
Moriyama and others (1969)	1023-1323	eqn	-242.096±0.344

Table A.05. Continued. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$Ni(s) + 0.5\ O_2(g) = NiO(bunsenite)$

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
Moser and others (1975)	1023-1273	eqn	-242.210±0.618
Myers and Gunter (1979)			
cooling	1079-1571	6	-238.630±1.022
heating	1072-1574	6	-238.638±0.996
* Oishi and others (1972)	1173-1273	eqn	-240.105±0.079
Ray and others (1984)	743-913	eqn	-240.536±0.101
	913-1323	eqn	-241.192±0.246
* Rog (1976)	873-1273	eqn	-239.665±0.395
Saito and others (1972)	1003-1263	eqn	-238.700±0.232
(also Saito, 1974)			
Schwab and Kustner (1981)	1044-1477	23	-238.623±0.831
* Sockel and Schmalzreid (1968)	1473	1	-240.917
Taylor and Schmalzreid (1964)	1073-1473	5	-237.897±1.449
Tran and Brungs (1880)	923-1573	14	-239.198±0.532
Treadwell (1916)	1253-1466	10	-281.546±2.200
* Tretyakov and Schmalzreid (1965)	1000-1500	eqn	-240.096±0.206
* Trumm (1971)	973-1273	4	-239.594±0.162

Table A.06. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

NiO(bunsenite) + CO(g) = Ni(s) + CO_2(g)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-42.703±0.372
Average of flagged studies below.			-42.778
* Antill and Warburton (1967)	850-1300	eqn	-42.358±0.311
Fricke and Weitbrecht (1942)	1044-1289	4	-40.717±0.143
* Klinedinst and Stevenson (1972)	923-1223	eqn	-42.172±0.240
Navrotsky and Muan (1970)	1323	1	-41.388
Peters and Mann (1958)	1173-1573	eqn	-45.251±0.098
* Tomlinson and Young (1964)	820-1120	eqn	-42.953±0.113
* Watanabe (1933)	936-1125	5	-43.630±0.129

Table A.07. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$NiO(bunsenite) + H_2(g) = Ni(s) + H_2O(g)$

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-1.549 ± 0.372
Average of flagged studies below.			-1.715
Babushkin and others (1971)	973-1273	8	(error in data)
* Gunter and others (1979)	852-1105 2 kb	6	-1.698 ± 0.789
* Pease and Cook (1926)	758-873	4	-1.975 ± 0.363
* Rau and Guedes de Carvalho (1973)	659-860	19	-1.471 ± 0.738

Table A.08. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

Cu_2O(cuprite) + Ni(s) = 2 Cu(s) + NiO(bunsenite)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-69.646±0.410
Average of flagged studies below.			-69.733
* Bidwell and Speiser (1963)	973-1298	eqn	-69.642±0.040
Bonnet and Perrin (1978)	1073-1273	eqn	-68.226±0.060
Bugden and Pratt (1970)	900-1400	eqn	-69.946±0.072
* Charette (1967)	969-1307	12	-69.522±0.034
Moriyama and others (1969)	973-1323	eqn	-69.812±0.018
	1023-1273	eqn	-69.438±0.036
	1073-1273	eqn	-70.098+0.036
Moser and others (1975)	973-1273	eqn	-70.030±0.180
O'Neill (1987)	797-1323	95	-70.154±0.096
* Pyun and Mueller (1977)	1075-1271	11	-69.796±0.148
Ramakrishnan and others (1975)	950-1250	eqn	-70.836±0.182
* Rizzo and others (1967)	973-1273	eqn	-69.826±0.021
* Sebkova and Baranek (1975)	1020-1400	4	-69.684±0.126
	1020-1323	17	-69.672±0.144
* Sellars and Maak (1966)	1073-1273	eqn	-69.666±0.096
* Shaiu and others (1977)	761-1092	45	-69.918±0.400
* Steele and Alcock (1965)	673-1273	eqn	-69.872±0.036
Trumm (1971)	973-1273	eqn	-70.138±0.036
Vasileva and others (1975)	1095-1228	eqn	-68.236±0.060

Table A.09. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$2\ CuO(tenorite) + Ni(s) = Cu_2O(cuprite) + NiO(bunsenite)$

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-99.589±0.573
Average of flagged studies below.			-99.348
* Charette (1967)	892-1320	15	-99.348±0.066

Table A.10. Calculated $\Delta_rH°(298)$ for observations within the wustite stability field. The following chemical reaction was considered:

$$2\ FeO(wus,sln) = 2\ Fe(wus,sln) + O_2(g).$$

In calculating the enthalpy of reaction, corrections were made for the activities of FeO(c) and Fe(c) according to the equations for those activities as given in the text. In each set of experiments one parameter was kept constant. This parameter is given in column 2. The first line shows the results from this study.

Source	Fixed Parameter	No. of Obs.	Method	$\Delta_rH°(298)$ (kJ/mol)
This evaluation (from weighted least-squares fit) - - - - -				524.266±0.822
<u>Data Given Weight in This Optimization</u>				
Average of weighted studies below - - - - - - - - - - - -				524.752
Ackermann and Sanford (1966)	T= 972	19	CO_2-CO mixtures, weight change	522.641±0.827
	=1023	19		525.337±0.656
	=1075	20		525.311±1.079
	=1182	21		525.691±0.581
	=1277	24		523.126±1.229
Branksy and Hed (1968)	T=1273.15	10	CO_2-CO mixtures, weight change	524.657±0.574
	=1373.15	15		524.999±0.528
	=1473.15	15		524.408±1.155
	=1573.15	15		524.482±1.095
Darken and Gurry (1945)	T=1373.15	5	CO_2-CO mixtures, chem. anal.	525.122±0.162
	=1473.15	5		524.995±0.209
	=1573.15	7		524.246±1.011
	=1623.15	8		524.335±0.945
	=1673.15	8		526.395±2.064
	CO_2/CO=-0.423	20		524.962±1.091
	=0.000	8		523.098±1.981
	=0.557	4		523.944±0.500
	=0.869	9		524.914±0.964
Gavarri and others (1979)	T=1258.15	8	CO_2-CO mixtures, previous results	525.736±0.684
	=1333.15	1		524.575
	=1348.15	8		525.199±1.101
Gerdanian and Dode (1965)	T=1073.15	15	CO_2-CO mixtures, weight change	524.438±0.796
Levin and Wagner (1967)	T=1273.15	23	CO_2-CO mixtures, weight change	525.987±1.481
Lohberg and Stannek (1955)	T=1173.15	5	H_2O-H_2 mixtures, chem. anal.	523.664±0.591
	=1273.15	8		523.497±0.367
	=1373.15	8		523.644±0.564
Marion (1955)	T= 905.15	2		523.276±0.246
	= 965.15	6		524.635±1.264
	=1083.15	12		524.772±0.674
	=1189.15	4		527.785±0.615
	=1273.15	5		528.026±0.243

Table A.10. Calculated $\Delta_r H°(298)$ for observations within the wustite stability field. Continued.

Source	Fixed Parameter	No. of Obs.	Method	$\Delta_r H°(298)$ (kJ/mol)
Riecke and Bohnenkamp (1969)	T=1073.15	3	H_2O-H_2 mixtures,	523.917±0.732
	=1173.15	8		523.684±0.592
	=1273.15	4		523.872±0.647
	=1373.15	7		524.054±0.958
Swaroop and Wagner (1967)	T=1223.15	10	CO_2-CO mixtures, weight change	524.453±0.544
	=1273.15	9		524.502±0.461
	=1323.15	5		524.547±0.387
	=1373.15	6		524.694±0.154
	=1423.15	5		524.719±0.240
	=1473.15	6		524.536±0.144
	=1523.15	6		524.031±0.617
Touzelin (1974)	T=1073.15	11	CO_2-CO mixtures, weight change	524.648±0.716
	=1173.15	13		523.414±0.596
	=1273.15	11		522.979±1.326
	=1348.15	18		522.327±0.320
Vallet and Raccah (1965)	T=1073.15	8	CO_2-CO mixtures, weight change	525.242±0.986
	=1093.15	16		525.147±0.980
	=1113.15	9		523.214±0.611
	=1123.15	10		525.586±0.681
	=1128.15	7		525.327±0.370
	=1133.15	15		524.989±0.684
	=1138.15	7		525.192±0.616
	=1143.15	9		525.112±0.529
	=1148.15	12		525.257±0.851
	=1153.15	10		525.547±1.100
	=1173.15	12		525.447±1.027
	=1193.15	9		525.033±1.107
	=1223.15	7		525.364±0.947
	=1273.15	7		524.611±0.689
	=1340.15	6		524.530±0.623
	=1395.15	8		524.308±0.938
	=1413.15	6		523.034±0.686
	=1433.15	7		522.759±1.411
	=1440.15	7		523.322±1.261
	=1473.15	7		523.788±0.754
	=1523.15	6		522.940±0.666

Table A.10. Calculated $\Delta_r H^\circ(298)$ for observations within the wustite stability field. Continued.

Source	Fixed Parameter	No. of Obs.	Method	$\Delta_r H^\circ(298)$ (kJ/mol)
<u>Data Given Zero Weight in This Optimization</u>				
Ariya and others (1954)	T=1104	8	CO_2-CO mixtures,	519.370±0.575
	=1182	7		518.874±0.763
Ariya and Yakovleva (1970)	x=0.069	3	emf using Fe/wus reference	527.171±0.347
	=0.086	4		526.848±0.247
	=0.095	6		526.220±0.045
	=0.097	6		527.133±0.142
	=0.104	7		526.478±0.101
	=0.112	6		526.260±0.107
	=0.121	4		526.610±0.107
	=0.125	6		526.631±0.221
	=0.134	5		525.423±0.180
	=0.146	1		525.979
Asao and others (1970)	x=0.068	4	emf using Ni/NiO reference	525.787±3.819
	=0.083	6		526.890±4.001
	=0.094	6		526.537±2.640
	=0.111	5		525.650±2.402
	=0.137	5		527.773±0.330
Barbero and others (1981)	x=0.049	4	emf using Ni/NiO refernce	523.948±1.220
	=0.056	6		521.553±2.787
	=0.074	6		520.803±1.260
	=0.083	5		519.653±1.017
	=0.091	5		520.211±0.969
	=0.096	5		519.120±0.968
	=0.103	4		518.070±1.152
	=0.121	3		516.023±1.004
	=0.124	2		518.529±1.262
Barbi (1964)	T= 973.15	4	emf using Fe/wus reference	518.632±0.585
	=1073.15	5		516.333±5.595
	=1173.15	7		519.417±2.149
Giddings (1972)	T=1253.15	11	emf, coulometry	523.052±0.071
	=1288.15	11		522.222±0.905
	=1296.15	11		522.009±0.916
	=1328.15	11		521.189±1.403
	=1348.15	11		521.763±1.123
	=1385.15	12		522.831±0.299
	=1385.15	12		523.176±0.312
Hauffe and Pfeiffer (1953)	T=1223.15	12	H_2O-H_2 mixtures, weight change	520.213±1.453
	=1273.15	12		521.506±1.034
Himmell and others (1953)	T=1073.15	5		523.918±2.873
	=1170.15	7		521.743±1.089
	=1256.15	10		519.805±1.529

Table A.10. Calculated $\Delta_rH^\circ(298)$ for observations within the wustite stability field. Continued.

Source	Fixed Parameter	No. of Obs.	Method	$\Delta_rH^\circ(298)$ (kJ/mol)
Janowski and others (1973)	T=1000	24	CO_2-CO mixtures, weight change	522.054±2.296
	=1025	24		523.617±2.203
	=1050	24		525.393±2.206
	=1100	24		529.229±2.081
	=1150	24		529.418±3.575
	=1200	24		533.180±2.662
	=1250	24		537.635±6.259
	=1300	24		539.771±5.252
	=1350	24		541.513±7.173
Katsura and Kimura (1965)	T=1433.15	3	CO_2-H_2 mixtures, chem. anal.	518.631±5.216
Marucco and others (1970)	T=1348.15	21	CO_2-CO mixtures, weight change	522.290±0.431
Myers and Eugster (1983)	T=1092.15	8	emf using air reference, weight change	517.442±1.372
	=1140.15	8		517.762±1.428
	=1194.15	7		515.533±0.885
	=1194.15	6		515.349±1.154
	=1198.15	3		517.170±0.904
	=1247.15	11		520.115±0.962
	=1273.15	4		524.914±5.673
	=1325.15	7		520.069±0.533
	=1326.15	9		518.612±1.530
	=1386.15	10		517.664±7.536
	=1429.15	12		517.901±1.086
	=1480.15	10		520.790±2.812
	=1536.15	13		523.591±4.858
Rizzo and Smith (1968)	T=1038.15	6	emf using air reference, coulometry	519.431±0.975
	=1138.15	7		521.210±0.411
	=1238.15	9		521.913±2.859

Table A.11. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$2\ FeO(wus,sln) = 2\ Fe(s) + O_2(g)$

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-524.266±0.822
Average of flagged studies below.			-523.687
Barbero and others (1981)	827-1323	eqn	-527.733±0.419
Fischer and Pateisky (1970)			
Stabilized Zirconia	943-1573	eqn	-525.484±0.632
Unstabilized Zirconia	800-1638	eqn	-522.176±2.600
Hahn and Muan (1962)	1373-1573	6	-529.729±3.497
* Holmes and others (1986)	837-1566	72	-524.608±0.330
* Jacobsson and Rosen (1981)	753-1554	-26	-523.132±0.776
Mallika and others (1986)	779-834	7	-523.002±0.080
Matsushita and Goto (1963)	773-1173	eqn	-522.130±1.260
Myers and Eugster (1983)	1088-1533	31	-517.376±1.824
Myers and Gunter (1978)			
cooling	1072-1575	6	-522.776±2.400
heating	1461-1570	3	-522.056±0.924
Rizzo (1968)	805-1476	156	-522.800±1.500
* Rog (1976)	873-1273	eqn	-521.960±1.400
* Schwab and Kuestner (1981)	1040-1415	18	-522.040±0.528
* Sockel and Schmalzreid (1968)	1473	1	-524.111
Sugimoto and others (1980)	873-1373	eqn	-524.020±1.900
* Takayama and Kimizuka (1980)	1373-1573	eqn	-525.785±0.741
* Taylor and Schmalzreid (1964)	1073-1473	5	-523.418±0.364
Treadwell (1916)	1213-1453	9	-562.788±4.100
* Tretyakov and Schmalzreid (1965)	1000-1500	eqn	-522.936±0.444
* Vallet 91965)	919-996	3	-525.199±0.605

Table A.12. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$FeO(wus,sln) + CO(g) = Fe(s) + CO_2(g)$

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-20.848±0.411
Average of flagged studies below.			-20.427
* Ariya and others (1954)	1104-1182	2	-20.812±0.042
Chaudron (1921)	838-1233	18	-20.645±2.128
* Darken and Gurry (1945)	1311-1648	8	-20.555±0.107
* Fakhoury and Rosenqvist (1978)	973-1173	eqn	-19.796±0.336
* Garran (1928)	923-1573	eqn	-20.159±0.442
* Golubenko and Rezukhina (1964)	1229-1472	12	-20.562±0.190
* Kiukkola and Wagner (1957)	1073-1273	4	-20.410±0.076
Kondakov and Wan (1958)	1173-1373	eqn	-20.341±0.072
* Marion (1955)	900-1400	eqn	-20.195±0.147
* Marucco and others (1970)	1348	1	-20.684
Matsubara (1922)	993-1351	8	-20.918±0.309
Peters and Mann (1959)	947-1519	7	-16.430±0.784
Peters and Mann (1958)	943-1523	eqn	-20.894±0.201
* Schenck and others (1927)			
Experiment # 1	873-1373	7	-20.249±0.165
Experiment # 2	813-1173	13	-19.891±0.640
* Schenck and others (1929)	873-1373	eqn	-20.406±0.116
* Schwerdtfeger and Muan (1966)	1273-1423	2	-20.390±0.057
* Schwerdtfeger and Muan (1967)	1273-1573	5	-20.394±0.160
* Touzelin (1974)	1073-1348	5	-20.355±0.554
* Vallet and Raccah (1965)	1053-1595	18	-21.548±0.824

Table A.13. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$FeO(wus,sln) + H_2(g) = Fe(s) + H_2O(g)$

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			20.306±0.411
Average of flagged studies below.			20.634
Britzke and others (1934)	1123-1498	eqn	19.231±0.613
Chaudron (1921)	855-1298	16	19.544±0.963
* Chipman and Marshall (1940)	1526-1633	4	20.756±0.140
Eastman and Evans (1924)	973-1273	eqn	17.517±0.408
Edmiston and Grace (1966)	1123-1224	6	22.113±0.308
* Emmett and Shultz (1930)	854-1293	42	20.687±0.224
* Emmett and Shultz (1933)	873-1273	10	20.615±0.254
* Jominy and Murphy (1931)	1364-1588	8	21.121±0.337
* Marion (1955)	900-1400	6	20.526±0.263
* Rau (1972)	860-978	11	20.359±0.086
Schreiner and Grimes (1920)			
H_2-controlled	903-1193	8	17.485±0.370
H_2O-controlled	868-1175	10	17.608±0.330
* Viktorovich and others (1972)	1073-1373	eqn	20.374±0.390
von Goldbeck (1949)	873-1223	eqn	21.908±0.561
Woehler and Balz (1921)	1148-1263	4	17.608±0.304
Woehler and Gunther (1923)	856-1282	24	17.248±0.903

Table A.14. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

Cu_2O(cuprite) + Fe(s) = 2 Cu(s) + FeO(wus,sln)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-91.501±0.469
Average of flagged studies below.			-91.263
Kiukkola and Wagner (1957)	1073-1323	eqn	-90.906±0.182
* Steele and Alcock (1965)	1073-1173	2	-91.263±0.084

Table A.15. Comparison of the third-law $\Delta_r H^\circ(298)$ from all studies with the results of this study for the reaction:

$NiO(bunsenite) + Fe(s) = Ni(s) + FeO(wus,sln)$

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H^\circ(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-21.855±0.554
Average of flagged studies below.			-21.790
Asao and others (1970)	880-1223	5	-20.700±0.276
* Bonnet and Perrin (1978)	1093-1273	eqn	-21.948±0.182
* Catlow and others (1977)	923-1523	eqn	-21.926±0.212
* Charette (1967)	903-1540	10	-21.748±0.214
* Davies and Smeltzer (1972)	873-1373	eqn	-21.646±0.184
Hoch and others (1962)	1386-1561	5	-19.374±0.210
* Jacobsson and Rosen (1981)	862-1619	72	-21.972±0.186
Kiukkola and Wagner (1957)	1023-1413	eqn	-21.638±0.042
* Levitsky and others (1965)	1185-1415	7	-21.736±0.128
Moriyama and others (1969)	1023-1373	eqn	-20.994±0.354
O'Neill (1987)	838-1416	122	-21.608±0.150
Pyun and Mueller (1977)	1075-1222	5	-21.176±0.308
Ramakrishnan and others (1975)	1173-1323	eqn	-21.332±0.860
* Rapp (1963)	973-1373	eqn	-21.818±0.400
* Roeder and Smeltzer (1964)	1003-1210	5	-21.512±0.510
* Saito and others (1972)	923-1373	eqn	-21.926±0.164
Sjoeden and others (1986)	866-1339	91	-22.398±0.138
Sreedharan and others (1977)	1033-1303	eqn	-20.288±0.878
* Steele and Alcock (1965)	973-1373	eqn	-21.668±0.096
Trumm (1971)	973-1273	4	-20.880±0.150

Table A.16. Comparison of the third-law $\Delta_r H^\circ(298)$ from all studies with the results of this study for the reaction:

$3\ Fe(s) + 2\ O_2(g) = Fe_3O_4$(magnetite)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H^\circ(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-1116.640±0.235
Average of flagged studies below.			-1118.370
* Humphrey and others (1952)	298.15	1	-1117.546
Mixter (1913)	298.15	1	-1111.420
Roth and Wienert (1934)	293.86	1	-1115.860
* Turnbull (1975)	298.20	4	-1117.200±2.000
Barbi (1964a)	773-850	5	-1116.354±1.213
Mallika and others (1986)	727-794	5	-1125.112±15.513
Matsushita and Goto (1963)	773-823	eqn	-1118.030±1.050
* Stofko and others (1974)	1473	1	-1120.453
Sugimoto and others (1980)	673-811	4	-1110.842+0.336

Table A.17. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$0.25\ Fe_3O_4$(magnetite) + CO(g) = 0.75 Fe(s) + CO_2(g)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-3.821±0.059
Marion (1955)	700-800	eqn	-2.917±0.033

Table A.18. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$0.25\ Fe_3O_4$(magnetite) + H_2(g) = 0.75 Fe(s) + H_2O(g)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			37.333±0.059
Average of flagged studies below.			37.614
Chaudron (1921)	738-763	4	36.673±0.382
	743-823	6	37.737±1.701
* Emmett and Shultz (1933)	674-823	36	37.831±0.334
Fricke and others (1941)	633-823	15	38.608±0.815
* Marion (1955)	700-800	eqn	37.810±0.044
* Rau (1972)	583-810	17	37.203±0.249
Woehler and Gunther (1923)	753-821	8	35.402±0.123

Table A.19. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$2\ Fe_3O_4(\text{magnetite}) = 6\ FeO(\text{wus,sln}) + O_2(g)$

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			660.485±2.511
Average of flagged studies below.			660.308
Barbero and others (1981)	827-1323	eqn	659.044±1.700
	827-1323	eqn	659.472±2.500
* Carel (1971)	1193-1624	21	659.833±0.701
Chizhikov and others (1969)	1500-1600	eqn	649.524±0.095
Chizhikov and others (1971)	1490-1600	eqn	564.574±2.145
* Gordeev (1966)	1173-1473	eqn	661.327±0.323
Myers and Eugster (1983)	1286-1553	12	658.692±3.696
Petric and others (1981)	1573	1	508.635
Rizzo (1968)			
Run 7	1077-1382	24	659.008±2.096
Run 12	1173-1473	24	661.712±3.464
Run 15	770-1321	102	654.784±6.488
* Schwab and Kuestner (1981)	1084-1459	15	658.296±0.621
Shchedrin and others (1978)	1450-1700	eqn	663.857±11.649
Snethlage and Klemm (1975)	1273-1473	3	659.043±1.416
* Snethlage and Schrocke (1976)	1273-1473	3	659.825±0.337
* Sockel and Schmalzreid (1968)	1473	1	659.858
* Takayama and Kimizuka (1980)	1373-1573	eqn	660.606±0.624
Treadwell (1916)	1223-1373	8	695.868±5.872
* Vallet (1965)	897-1210	4	662.4884±2.524

Table A.20. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

Fe_3O_4(magnetite) + Fe(s) = 4 FeO(wus,sln)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			68.110±1.661
Average of flagged studies below.			67.943
* Ariya and Yakovleva (1970)	1162-1311	10	67.112±0.536
* Barbi (1964a)	842.15	1	68.856
* Birks (1966)	843.15	1	67.864
* Eremenko and Filippov (1967)	1123-1423	eqn	66.200±1.984
Gordeev and Tretyakov (1963)	1173-1373	3	69.072±1.640
Hoch and others (1962)	1173-1440	7	96.432±13.016
* Jacobsson (1965)	960-1602	108	68.048±0.800
* Kiukkola and Wagner (1957)	1073-1373	eqn	68.384±0.744
* Levitsky and others (1965)	1186.1573	18	69.048±2.696
Moriyama and others (1969)	1073-1273	eqn	69.800±0.280
* Roeder and Smeltzer (1964)	1073-1273	4	68.032±0.344
Trumm (1971)	973-1273	eqn	75.384±4.408

Table A.21. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

Fe_3O_4(magnetite) + CO(g) = 3 FeO(wus,sln) + CO_2(g)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			47.262±1.256
Average of flagged studies below.			47.489
* Ariya and others (1954)	1104-1182	2	48.276±0.693
Chaudron (1921)	883-1273	14	48.723±4.545
* Darken and Gurry (1945)	1396-1661	5	46.926±0.414
Eastman and Evans (1924)	1091-1312	9	48.679±0.569
* Fakhoury and Rosenqvist (1978)	973-1173	eqn	47.722±1.529
* Garran (1928)	873-1523	eqn	47.986±0.868
* Kiukkola and Wagner (1957)	1073-1373	4	47.584±0.170
* Marion (1955)	900-1400	eqn	48.409±0.520
Marucco and others (1970)	1348	1	47.512
Matsubara (1922)	900-1343	5	48.219±0.307
* Petric and others (1981)	1573	1	46.634
Schenck and others (1927)			
Experiment # 1	873-1373	7	47.229±0.386
Experiment # 2	813-1173	8	47.175±0.504
* Schwerdtfeger and Muan (1966)	1273-1473	3	47.101±0.067
* Schwerdtfeger and Muan (1967)	1423-1573	3	46.920±0.070
* Touzelin (1974)	1173-1348	3	47.451±0.624
Trinel-Dufour and Perrot (1977)	1273	1	48.066
* Vallet and Raccah (1965)	1133-1398	10	47.375±0.426

Table A.22. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

Fe_3O_4(magnetite) + H_2(g) = 3 FeO(wus,sln) + H_2O(g)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			88.416±1.256
Average of flagged studies below.			88.822
Bulgakova and Zaitsev (1965)	1250	1	90.688
Chaudron (1921)	843-1078	14	89.344±1.569
Eastman and Evans (1924)	973-1273	eqn	86.812±0.101
* Emmett and Shultz (1930)	970-1075	13	88.701±0.307
* Emmett and Shultz (1933)	872-1075	17	88.695±0.207
* Marion (1955)	900-1400	eqn	89.315±0.316
* Rau (1972)	859-882	5	88.542±0.225
* Viktoyorvich and others (1972)	1073-1373	eqn	88.861±1.010
Woehler and Balz (1921)	998-1223	8	87.739±2.201
Woehler and Gunther (1923)	902-1186	12	86.772±0.637

Table A.23. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

Fe_3O_4(magnetite) + 2 Cu(s) = 3 FeO(wus,sln) + Cu_2O(cuprite)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			159.612±1.277
Kiukkola and Wagner (1957)	1073-1323	7	159.162±1.086

Table A.24. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

Fe_3O_4(magnetite) + Ni(s) = 3 FeO(wus,sln) + NiO(bunsenite)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			89.965±1.312
Average of flagged studies below.			89.480
Asao and others (1970)	985-1273	6	89.734±0.982
* Bonnet and Perrin (1978)	1073-1273	eqn	89.582±0.260
* Charette (1967)	949-1272	12	89.882±0.132
* Roeder and Smeltzer (1964)	923-1273	4	89.270±0.358
* Saito and others (1972)	1043-1353	8	89.186±0.126

Table A.25. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$2\ Fe(s) + 1.5\ O_2(g) = Fe_2O_3$(hematite)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-824.928±0.149
Mixter (1913)	298.15	1	-804.030
Roth and Wienert (1934)	293.86	1	-816.496

Table A.26. Comparison of the third-law $\Delta_r H^\circ(298)$ from all studies with the results of this study for the reaction:

$2\ Fe_3O_4(\text{magnetite}) + 0.5\ O_2(g) = 3\ Fe_2O_3(\text{hematite})$

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H^\circ(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-241.506±0.705
Average of flagged studies below.			-241.694
Chizhikov and others (1971)	1030-1200	8	-272.160±10.357
* Darken and Gurry (1946)	1586-1730	3	-242.291±0.574
* Komarov and others (1967)	1526-1657	4	-242.099±0.377
* Kurepin (1975)	1473-1573	2	-241.669±0.429
Myers and Eugster (1983)	1321-1888	9	-240.272±0.952
Norton (1955)	1057-1342	8	-239.311±1.098
* Schmahl (1941)	1583-1683	6	-242.414±0.154
Schmahl and others (1969)	1448-1698	eqn	-239.459±1.098
Schwab and Kuestner (1981)	1129-1340	14	-239.339±0.597
* Smiltens (1957)	1452-1731	4	-242.229±0.979
* Snethlage and Schrocke (1976)	1273-1473	3	-241.021±0.319
Treadwell (1916)	1253-1353	6	-227.366+1.946
Tretyakov and Khomyakov (1962)	1373-1728	eqn	-236.136±1.394
* Tretyakov and others (1977)	1423-1623	eqn	-240.140±0.212
White and Richards (1949)	1641-1673	3	-237.575±0.965

Table A.27. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$3\ Fe_2O_3(\text{hematite}) + H_2(g) = 2\ Fe_3O_4(\text{magnetite}) + H_2O(g)$

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-0.320±0.702
Average of flagged studies below.			-1.485
* Rau (1972)	767-840	6	-1.485±0.812
Woehler and Balz (1921)	793-1073	4	-1.549±3.744
Woehler and Gunther (1923)	623.15	4	0.005±1.155

Table A.28. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$3\ Fe_2O_3$(hematite) + 2 Cu(s) = $2\ Fe_3O_4$(magnetite) + Cu_2O(cuprite)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			70.875±0.728
Average of flagged studies below.			70.601
Bonnet and Perrin (1978)	1123-1273	eqn	69.570±0.706
* Bryant and Smeltzer (1969)	1059-1323	33	70.660±0.314
* Fitzner (1979)	1091-1261	8	70.376±0.916
* Ramana Rao and Tare (1972)	1165-1280	8	70.566±0.200
* Ramana Rao and Tare (1973)	915-1310	11	70.802±0.222

Table A.29. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$3\ Fe_2O_3$(hematite) + Ni(s) = $2\ Fe_3O_4$(magnetite) + NiO(bunsenite)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			1.229±0.790
Average of flagged studies below.			1.058
* Charette (1967)	967-1373	16	1.132±0.182
Moriyama and others (1969)	1073-1273	eqn	3.114±0.344
Saito and others (1972)	1073-1343	eqn	0.378±0.050
(also Saito, 1974)			
* Trumm (1981)	1196-1269 2-7 kb	6	0.984±0.196
Ulmer and others (1976)	973-1573 34 kb	11	-7.640±0.920

Table A.30. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

3 Fe_2O_3(hematite) + Fe(s) = 2 Fe_3O_4(magnetite) + FeO(wus,sln)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-20.626±0.972
Average of flagged studies below.			-20.684
Blumenthal (1961)	1073-1323	eqn	-18.046±0.780
Gordeev and Tretyakov (1963)	1073-1373	eqn	-17.350±2.122
* Jacobsson (1985)	1088-1592	66	-20.684±0.352

Table A.31. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

Fe_2SiO_4(fayalite) = Fe_2SiO_4(spinel structure)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			6.767±3.064
Average of flagged studies below.			6.623
* Navrotsky and others (1979)	986.15	1	6.674±1.167
Akimoto and Fujisawa (1965)	1083-1243 46-59 kb	2 pr	7.468±1.920
* Akimoto and others (1967)	1028-1768 44-63 kb	7 pr	6.321±1.015
Akimoto and others (1977)	973-1393 51-63 kb	2 pr	9.556±0.313
Akimoto and Yagi (1986)	1073-1473 47-58 kb	eqn	6.626±0.159
Ohtani and others (1979)	1838-1878 71-73 kb	1 pr	10.388±0.616

Table A.32. Comparison of the enthalpy of melting, $\Delta_m H^\circ$, from all studies with the results of this study for the reaction:

Fe_2SiO_4(fayalite) = Fe_2SiO_4(liquid)

Source	Temperature Range K	Number of Obs.	$\Delta_m H^\circ(1490)$ kJ/mol
This evaluation (from weighted least-squares fit)			88.049±2.315
Average of flagged studies below.			88.709
* Stebbins and Carmichael (1984)	1490	1	89.300±1.100
* Akimoto and others (1967)	1548-1809 17-62 kb	7 pr	88.560±1.936
* Hsu (1967)	1523-1678 10-40 kb	7 pr	87.621±0.780
Kato and others (1984)	1668-1678	1 pr	79.404±0.365
* Lindsley (1967)	1515-1719 10-40 kb	4 pr	89.353±1.325
Ohtani (1979)	1898-1998 64-71 kb	2 pr.	95.191±4.000

Table A.33. Comparison of the enthalpy of melting, $\Delta_m H°$, from all studies with the results of this study for the reaction:

Fe_2SiO_4(spinel structure) = Fe_2SiO_4(liquid)

The estimated melting temperature at 1 bar total pressure is 1090±40 K.

Source	Temperature Range K	Number of Obs.	$\Delta_m H°(1090)$ kJ/mol
This evaluation (from weighted least-squares fit)			70.299±4.060
Average of flagged studies below.			70.358
* Akimoto and others (1967)	1758-1983 62-76 kb	2 pr	70.358±3.622
Ohtani (1979)	1858-2613 77-130 kb	6 pr.	73.003±10.000

Table A.34. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$2\ Fe(s) + Si(s) + 2\ O_2(g) = Fe_2SiO_4$(fayalite)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-1477.733±1.324
King (1952)	298.15	1	-1479.706±1.900

Table A.35. Comparison of the third-law $\Delta_rH°(298)$ from all studies with the results of this study for the reaction:

Fe_2SiO_4(fayalite) = 2 Fe(s) + SiO_2(quartz) + O_2(g)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_rH°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			567.031±1.324
Average of flagged studies below.			563.678
* Kitayama and Katsura (1968)	1402-1447	4	563.419±1.032
Myers and Eugster (1983)	1241-1405	12	557.428±1.448
Nafziger and Muan (1967)	1423	1	548.642
	1473	1	537.215
* Schwab and Kustner (1981)	1099-1414	12	563.600±0.771
* Taylor and Schmalzreid (1964)	1173-2743	3	564.015±0.938
Williams (1971)	1198-1451	4	560.917±6.061

Table A.36. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$0.5\ Fe_2SiO_4$(fayalite) + CO(g) = Fe(s) + 0.5 SiO_2(quartz) + CO_2(g)

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			0.535±0.662
Average of flagged studies below.			0.792
* Lebedev and Levitsky (1962)	1123-1423	17	0.992±0.501
* Schenck and others (1932)	1173	1	0.548
* Schwerdtfeger and Muan (1966)	1273-1423	3	0.836±0.200

Table A.37. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$0.5\ Fe_2SiO_4(\text{fayalite}) + H_2(g) = Fe(s) + 0.5\ SiO_2(\text{quartz}) + H_2O(g)$

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			41.689±0.662
Berliner and Shapovolova (1966)	1033-1403	13	46.034±1.550

Table A.38. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

FeO(wus,sln) + 0.5 SiO_2(quartz) = 0.5 Fe_2SiO_4(fayalite)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-21.383±0.780
Average of flagged studies below.			-21.072
* Levitsky and Ratiani (1970)	1104-1269	17	-21.072±0.230
O'Neill (1987)	971-1268	61	-20.998±0.178
Shiomi and others (1975)	973-1223	eqn	-21.072±0.174

Table A.39. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

$$2\ Fe(s) + SiO_2(quartz) + 2\ Fe_3O_4(magnetite)$$
$$= Fe_2SiO_4(fayalite) + 6\ FeO(wus,sln)$$

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			93.545±2.840
Eremenko and Filippov (1967)	1223-1423	eqn	error in data

Table A.40. Comparison of the third-law $\Delta_r H^\circ(298)$ from all studies with the results of this study for the reaction:

$2\ Fe_3O_4(\text{magnetite}) + 3\ SiO_2(\text{quartz}) = 3\ Fe_2SiO_4(\text{fayalite}) + O_2(g)$

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H^\circ(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			532.187±4.005
Muan (1955)	1413	1	528.969
Myers and Eugster (1983)	1391-1406	2	530.567±0.273
Schwab and Kuestner (1981)	1007-1181	24	540.702±6.703
	1191-1431	42	529.647±1.200
Schwab and Sohnlein (1971)	1308-1403	6	539.052±3.600

Table A.41. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

Fe_3O_4(magnetite) + 1.5 SiO_2(quartz) + CO(g)

= 1.5 Fe_2SiO_4(fayalite) + CO_2(g)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-16.887±2.003
Average of flagged studies below.			-14.667
Schenck and others (1932)	1173	1	-12.923
* Schwerdtfeger and Muan (1966)	1373	1	-14.667

Table A.42. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

Fe_3O_4(magnetite) + 1.5 SiO_2(quartz) + H_2(g)

= 1.5 Fe_2SiO_4(fayalite) + H_2O(g)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			24.266±2.003
Average of flagged studies below.			23.456
* Hewitt (1978)	925-1128 1 kb	8	24.141±0.730
* Myers and Eugster (1983)	927-1038 1 kb	12	22.771±0.851
Wones and Gilbert (1969)	867-1076 1 and 2 kb	16	28.284±0.551

Table A.43. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

Fe_3O_4(magnetite) + 1.5 SiO_2(quartz) + 2 Cu(s)

= 1.5 Fe_2SiO_4(fayalite) + Cu_2O(cuprite)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			-95.462±2.016
O'Neill (1987)	1049-1311	38	-96.900±0.166

Table A.44. Comparison of the third-law $\Delta_r H°(298)$ from all studies with the results of this study for the reaction:

Fe_3O_4(magnetite) + 1.5 SiO_2(quartz) + Fe(s)

= 1.5 Fe_2SiO_4(fayalite) + FeO(wus,sln)

The pressure was 1.01 bars (nominal) unless otherwise indicated. Data sets flagged with an asterisk (*) were used in this study.

Source	Temperature Range K	Number of Obs.	$\Delta_r H°(298)$ kJ/mol
This evaluation (from weighted least-squares fit)			3.906±2.044
Schwab and Sohnlein (1977)	1303-1378	4	3.878±1.048

Table B.1. Fitted constants for use in equations. They are arranged alphabetically by chemical formula. The constants for the empirical functions a(T), a'(T), b(T), r(T), and s(T) are given last.

Phase	C(s)	CO(g)	$CO_2(g)$	Cu(s)
	Graphite			Copper
$a_{1,i}$	$-5.460481x10^{7}$	$1.353359x10^{8}$	$-2.358936x10^{7}$	$-1.152049x10^{8}$
$a_{2,i}$	$6.956641x10^{5}$	$-3.207182x10^{6}$	---	$3.110370x10^{6}$
$a_{3,i}$	$6.129584x10^{3}$	$4.491154x10^{4}$	$1.278701x10^{4}$	$-5.196059x10^{4}$
$a_{3,i}$	$-1.531500x10^{3}$	$-3.323073x10^{3}$	$-1.910433x10^{3}$	$4.211849x10^{3}$
$a_{5,i}$	74.69532	$1.042867x10^{2}$	$1.074207x10^{2}$	-84.53039
$a_{6,i}$	$-1.336926x10^{-2}$	$-7.883444x10^{-3}$	$-5.466799x10^{-3}$	$2.909935x10^{-2}$
$a_{7,i}$	$1.968607x10^{-6}$	---	---	---
$a_{8,i}$	---	---	---	---
$a_{9,i}$	8.257652	$-2.601026x10^{5}$	$-3.694304x10^{5}$	$1.941727x10^{5}$
$a_{10,i}$	$-5.695527x10^{2}$	$-6.447801x10^{2}$	$-5.753145x10^{2}$	$8.357028x10^{2}$
$a_{11,i}$	---	---	---	---
$a_{12,i}$	---	---	---	---
$a_{13,i}$	---	---	---	---
$a_{14,i}$	---	---	---	---
j'_i	---	---	---	---
j''_i	---	---	---	---
n_i	---	---	---	---
$b_{1,i}$	---	---	---	---
$b_{2,i}$	---	---	---	---
$b_{3,i}$	---	---	---	---
$b_{4,i}$	---	---	---	---
$b_{5,i}$	---	---	---	---

Table B.1 Continued. Fitted constants for use in equations.

Phase	Cu(l)	CuO(s) Tenorite	Cu_2O(s) Cuprite	Cu_2O(l)
$a_{1,i}$	---	---	---	---
$a_{2,i}$	---	1.428191×10^{6}	1.254170×10^{6}	---
$a_{3,i}$	---	-4.209052×10^{4}	-3.539570×10^{4}	---
$a_{3,i}$	---	3.287230×10^{3}	2.734785×10^{3}	---
$a_{5,i}$	32.80000	-30.19985	---	99.61357
$a_{6,i}$	---	2.204283×10^{-2}	2.927305×10^{-2}	---
$a_{7,i}$	---	---	---	---
$a_{8,i}$	---	---	---	---
$a_{9,i}$	8.124944×10^{3}	2.349399×10^{4}	-1.017000×10^{4}	-1.089787×10^{5}
$a_{10,i}$	-1.526609×10^{2}	4.527213×10^{2}	2.887472×10^{2}	-4.705172×10^{2}
$a_{11,i}$	---	2.270000×10^{2}	---	---
$a_{12,i}$	---	---	---	---
$a_{13,i}$	---	2.192563	---	---
$a_{14,i}$	---	1.920467	---	---
j_i'	---	1	---	---
j_i''	---	5	---	---
n_i	---	7	---	---
$b_{1,i}$	---	---	---	---
$b_{2,i}$	---	---	---	---
$b_{3,i}$	---	---	---	---
$b_{4,i}$	---	---	---	---
$b_{5,i}$	---	---	---	---

Table B.1 Continued. Fitted constants for use in equations.

Phase	Fe(α) Iron	Fe(γ) Iron	FeO(s)	Fe_2O_3(s) Hematite
$a_{1,i}$	-3.164859×10^{8}	---	5.684245×10^{7}	---
$a_{2,i}$	6.760865×10^{6}	---	-9.718540×10^{5}	3.733780×10^{6}
$a_{3,i}$	-9.231270×10^{4}	---	-1.692931×10^{3}	-9.713516×10^{4}
$a_{3,i}$	6.807541×10^{3}	---	4.374162×10^{2}	6.544510×10^{3}
$a_{5,i}$	-1.350233×10^{2}	24.00467	33.75275	---
$a_{6,i}$	3.661824×10^{-2}	8.325572×10^{-3}	9.728070×10^{-3}	2.777694×10^{-2}
$a_{7,i}$	---	---	---	---
$a_{8,i}$	---	---	---	---
$a_{9,i}$	3.585077×10^{5}	8.399285×10^{3}	-2.430891×10^{5}	-3.782323×10^{5}
$a_{10,i}$	1.298501×10^{3}	-1.037138×10^{2}	-96.60265	5.321845×10^{2}
$a_{11,i}$	1.042000×10^{3}	---	1.900000×10^{2}	9.555300×10^{2}
$a_{12,i}$	---	---	2.163000×10^{-3}	---
$a_{13,i}$	17.60583	---	11.07758	25.74863
$a_{14,i}$	13.65770	---	8.316250	17.60611
j_i'	3	---	3	3
j_i''	5	---	15	15
n_i	15	---	7	7
$b_{1,i}$	6.777561	6.479734	11.85631	29.75927
$b_{2,i}$	3.869045×10^{-4}	5.176589×10^{-4}	6.171253×10^{-4}	1.300762×10^{-3}
$b_{3,i}$	1.214274×10^{-1}	3.623244×10^{-1}	3.690561×10^{-1}	4.810625×10^{-1}
$b_{4,i}$	-3.328568×10^{-7}	-3.010978×10^{-7}	-5.395723×10^{-7}	-4.600481×10^{-7}
$b_{5,i}$	2.178608×10^{-2}	2.783103×10^{-2}	4.558140×10^{-3}	-1.641547×10^{-3}

Table B.1 Continued. Fitted constants for use in equations.

Phase	$Fe_2SiO_4(s1)$ Fayalite	$Fe_2SiO_4(s2)$	$Fe_2SiO_4(l)$	$Fe_3O_4(s)$ Magnetite
$a_{1,i}$	---	---	---	-1.124245×10^{9}
$a_{2,i}$	1.992984×10^{6}	-4.418744×10^{5}	---	2.516752×10^{7}
$a_{3,i}$	-3.779270×10^{4}	---	---	-3.315259×10^{5}
$a_{3,i}$	3.109141×10^{2}	-1.725535×10^{3}	---	2.118956×10^{4}
$a_{5,i}$	2.207439×10^{2}	2.364687×10^{2}	2.268339×10^{2}	-2.256132×10^{2}
$a_{6,i}$	-8.036396×10^{-3}	1.385994×10^{-3}	---	6.483540×10^{-2}
$a_{7,i}$	---	---	---	---
$a_{8,i}$	---	---	---	---
$a_{9,i}$	-1.187687×10^{6}	-1.339194×10^{6}	-1.371166×10^{6}	3.296806×10^{5}
$a_{10,i}$	-1.183900×10^{3}	-1.410438×10^{3}	-1.172471×10^{3}	2.881133×10^{3}
$a_{11,i}$	---	---	---	8.491000×10^{2}
$a_{12,i}$	---	---	---	2.002913×10^{-3}
$a_{13,i}$	---	---	---	63.83825
$a_{14,i}$	---	---	---	47.56546
j'_i	---	---	---	4
j''_i	---	---	---	15
n_i	---	---	---	7
$b_{1,i}$	44.89739	42.00207	50.39495	42.93467
$b_{2,i}$	1.662934×10^{-3}	2.852301×10^{-4}	---	2.731470×10^{-3}
$b_{3,i}$	4.422591×10^{-1}	-1.015284	---	1.261525
$b_{4,i}$	-4.941970×10^{-7}	-3.515602×10^{-7}	---	-3.860242×10^{-7}
$b_{5,i}$	1.343700×10^{-2}	8.745524×10^{-3}	8.007576×10^{-3}	7.372981×10^{-3}

Table B.1 Continued. Fitted constants for use in equations.

Phase	$H_2(g)$	$H_2O(s)$	$H_2O(l)$	$H_2O(g)$
		Ice		
$a_{1,i}$	2.128797×10^{8}	---	---	---
$a_{2,i}$	-3.226409×10^{6}	-9.327362×10^{5}	---	-1.183031×10^{6}
$a_{3,i}$	2.413888×10^{4}	4.609950×10^{4}	6.246402×10^{4}	2.497038×10^{4}
$a_{3,i}$	-1.163430×10^{3}	-5.931491×10^{3}	-8.094280×10^{3}	-1.972216×10^{3}
$a_{5,i}$	42.49826	2.403792×10^{2}	3.626257×10^{2}	76.23971
$a_{6,i}$	3.400246×10^{-3}	---	-9.396194×10^{-2}	3.853708×10^{-3}
$a_{7,i}$	---	---	---	---
$a_{8,i}$	---	---	---	---
$a_{9,i}$	-8.083936×10^{4}	-3.557653×10^{5}	-3.965432×10^{5}	-2.733140×10^{5}
$a_{10,i}$	-1.817369×10^{2}	-1.862466×10^{3}	-2.696170×10^{3}	-3.980379×10^{2}
$a_{11,i}$	---	---	---	---
$a_{12,i}$	---	---	---	---
$a_{13,i}$	---	---	---	---
$a_{14,i}$	---	---	---	---
j'_i	---	---	---	---
j''_i	---	---	---	---
n_i	---	---	---	---
$b_{1,i}$	---	---	---	---
$b_{2,i}$	---	---	---	---
$b_{3,i}$	---	---	---	---
$b_{4,i}$	---	---	---	---
$b_{5,i}$	---	---	---	---

Table B.1 Continued. Fitted constants for use in equations.

Phase	Ni(s)	Ni(l)	NiO(s)	O_2(g)
	Nickel		Bunsenite	
$a_{1,i}$	$2.695368\text{x}10^{7}$	---	---	$-3.442864\text{x}10^{8}$
$a_{2,i}$	---	---	$4.203972\text{x}10^{6}$	$4.573348\text{x}10^{6}$
$a_{3,i}$	$-1.121795\text{x}10^{4}$	---	$-9.437250\text{x}10^{4}$	$-2.898726\text{x}10^{4}$
$a_{3,i}$	$1.111718\text{x}10^{3}$	---	$7.138737\text{x}10^{3}$	$1.133732\text{x}10^{3}$
$a_{5,i}$	-6.479189	38.95234	$-1.106966\text{x}10^{2}$	21.91898
$a_{6,i}$	$1.440432\text{x}10^{-2}$	---	$3.142742\text{x}10^{-2}$	$1.854499\text{x}10^{-3}$
$a_{7,i}$	---	---	---	---
$a_{8,i}$	---	---	---	---
$a_{9,i}$	$3.586014\text{x}10^{4}$	$-6.136540\text{x}10^{3}$	$1.359868\text{x}10^{5}$	$1.939566\text{x}10^{5}$
$a_{10,i}$	$1.538951\text{x}10^{2}$	$-1.946085\text{x}10^{2}$	$1.191473\text{x}10^{3}$	$1.352015\text{x}10^{2}$
$a_{11,i}$	$6.310000\text{x}10^{2}$	---	$5.190000\text{x}10^{2}$	---
$a_{12,i}$	$2.753421\text{x}10^{-4}$	---	---	---
$a_{13,i}$	4.272993	---	8.506945	---
$a_{14,i}$	2.567885	---	8.109302	---
j'_i	3	---	3	---
j''_i	5	---	15	---
n_i	15	---	7	---
$b_{1,i}$	6.416513	5.664487	10.65752	---
$b_{2,i}$	$3.590238\text{x}10^{-4}$	$1.023200\text{x}10^{-3}$	$5.014680\text{x}10^{-4}$	---
$b_{3,i}$	$8.749865\text{x}10^{-2}$	---	$8.496485\text{x}10^{-2}$	---
$b_{4,i}$	$-5.025971\text{x}10^{-7}$	---	$-3.425463\text{x}10^{-7}$	---
$b_{5,i}$	---	---	$1.365322\text{x}10^{-2}$	---

Table B.1 Continued. Fitted constants for use in equations.

Phase	Si(s)	Si(l)	SiO_2(s1,α) α-Quartz	SiO_2(s2,β) β-Quartz
$a_{1,i}$	---	---	8.750792×10^{7}	---
$a_{2,i}$	-1.480200×10^{5}	---	-1.958203×10^{6}	8.216362×10^{6}
$a_{3,i}$	---	---	3.672359×10^{4}	---
$a_{3,i}$	-1.771890×10^{2}	---	-4.248991×10^{3}	-7.281991×10^{2}
$a_{5,i}$	31.70500	25.52240	1.901032×10^{2}	74.52595
$a_{6,i}$	5.627460×10^{-4}	---	-1.303393×10^{-2}	9.154193×10^{-3}
$a_{7,i}$	---	---	---	---
$a_{8,i}$	---	---	---	---
$a_{9,i}$	1.752952×10^{3}	4.906151×10^{4}	-9.686044×10^{5}	-8.232235×10^{5}
$a_{10,i}$	-1.833560×10^{2}	-97.81430	-1.416686×10^{3}	-4.496128×10^{2}
$a_{11,i}$	---	---	8.455000×10^{2}	---
$a_{12,i}$	---	---	2.612794×10^{-2}	---
$a_{13,i}$	---	---	16.07524	---
$a_{14,i}$	---	---	---	---
j'_i	---	---	---	---
j''_i	---	---	---	---
n_i	---	---	---	---
$b_{1,i}$	---	---	21.00329	21.23888
$b_{2,i}$	---	---	1.483792×10^{-3}	---
$b_{3,i}$	---	---	5.533663×10^{-1}	-1.394691
$b_{4,i}$	---	---	-1.220384×10^{-6}	8.539966×10^{-7}
$b_{5,i}$	---	---	4.850748×10^{-2}	1.187518×10^{-1}

Table B.1 Continued. Fitted constants for use in equations.

Phase	SiO_2(s3,α) α-Cristobalite	SiO_2(s4,β) β-Cristobalite	O_2(i-w)=a(T)	O_2(i'-w)=a'(T)
$a_{1,i}$	---	---	---	---
$a_{2,i}$	4.321152×10^{5}	-4.143189×10^{6}	---	---
$a_{3,i}$	---	---	---	---
$a_{3,i}$	-1.508734×10^{3}	---	-6.097747×10^{3}	---
$a_{5,i}$	1.316256×10^{2}	72.77177	2.843665×10^{2}	-17.07577
$a_{6,i}$	-1.413170×10^{-2}	1.290805×10^{-3}	-8.678193×10^{-2}	---
$a_{7,i}$	---	---	---	---
$a_{8,i}$	---	---	---	---
$a_{9,i}$	-8.263396×10^{5}	-8.740686×10^{5}	6.705241×10^{5}	5.508655×10^{5}
$a_{10,i}$	-8.746669×10^{2}	-3.882548×10^{2}	-2.135301×10^{3}	2.528698×10^{2}
$a_{11,i}$	---	---	---	---
$a_{12,i}$	---	---	---	---
$a_{13,i}$	---	---	---	---
$a_{14,i}$	---	---	---	---
j_i'	---	---	---	---
j_i''	---	---	---	---
n_i	---	---	---	---
$b_{1,i}$	23.44202	25.21268	---	---
$b_{2,i}$	1.121859×10^{-3}	---	---	---
$b_{3,i}$	-7.736267×10^{-1}	-1.445465	---	---
$b_{4,i}$	---	---	---	---
$b_{5,i}$	9.625593×10^{-2}	9.162409×10^{-2}	---	---

Table B.1 Continued. Fitted constants for use in equations.

Phase	O_2(w-m)=b(T)	r(T)	s(T)
$a_{1,i}$	---	---	---
$a_{2,i}$	$-4.205002\text{x}10^{7}$	---	---
$a_{3,i}$	---	---	---
$a_{3,i}$	$3.601333\text{x}10^{4}$	---	---
$a_{5,i}$	$-1.866786\text{x}10^{3}$	$-1.026279\text{x}10^{2}$	---
$a_{6,i}$	$7.581317\text{x}10^{-1}$	$-2.721420\text{x}10^{-2}$	$1.684236\text{x}10^{-1}$
$a_{7,i}$	---	---	---
$a_{8,i}$	---	---	---
$a_{9,i}$	$-2.076200\text{x}10^{5}$	$6.836500\text{x}10^{5}$	---
$a_{10,i}$	$1.463965\text{x}10^{4}$	$8.792671\text{x}10^{2}$	$3.323205\text{x}10^{2}$
$a_{11,i}$	---	---	---
$a_{12,i}$	---	---	---
$a_{13,i}$	---	---	---
$a_{14,i}$	---	---	---
j'_i	---	---	---
j''_i	---	---	---
n_i	---	---	---
$b_{1,i}$	---	---	---
$b_{2,i}$	---	---	---
$b_{3,i}$	---	---	---
$b_{4,i}$	---	---	---
$b_{5,i}$	---	---	---

Table B.2. Equations used to calculate thermodynamic properties in standard conventions.

Property	Symbol	Equation	Comments
Heat Capacity	$C^\circ_{P,i}$	5.30,5.31	
Entropy	$S^\circ_i(T,P)$	5.32	
Enthalpy	$h^\circ_i(T,P)$	5.36	
	$\Delta_f H^\circ$	5.43	Replace G and g by H and h.
	$\Delta_r H^\circ$	----	= $\Sigma n_i h^\circ_i$ where n_i is the stoichiometric coefficient.
	$H^\circ_i(T)-H^\circ_i(Tr)$	5.36	Evaluate at T and Tr. Then take difference.
Gibbs energy	$g^\circ_i(T,P)$	5.40	
	$\Delta_f G^\circ$	5.43	
	$\Delta_r G^\circ$	----	= $\Sigma n_i g^\circ_i$ where n_i is the stoichiometric coefficient.
Gibbs energy function	$gef^\circ_i(T)$	7.44	
log activity	log a(i)	5.45	
Equilibrium constant	log K°	5.07	
Electrochemical potential	E°	5.08	
Volume	V(T,P)	5.13	
	V(T)/V(Tr)	5.13	Evaluate at T and Tr. Then take ratio.
	[V(T)-V(Tr)]/V(Tr)	5.13	Evaluate at T and Tr. Then take difference and ratio.
Coefficient of volume expansion	α	5.15	
	"α"	5.17	= [V(T)-V(Tr)]/[V(Tr)x(T-Tr)]
Coefficient of volume compression	β	5.19	
	"β"	5.21	= [V(T)-V(Tr)]/[V(Tr)x(T-Tr)]
Critical or Neel temperature	T_C or T_N	5.29	

Table B.3. Equations used to calculate thermodynamic properties of wustite, $Fe_{1-y}O$ or FeO_{1+x}, in standard conventions. The notation FeO(wus,sln) is used sometimes in the text and tables.

Property	Symbol	Equation	Comments
Heat Capacity	$C^\circ_{P,i}$	5.67	Refer to Table B.2 for $C^\circ_p(FeO)$
Entropy	$S^\circ_i(T,P)$	5.69	Refer to Table B.2 for $S^\circ(FeO)$
Enthalpy	$h^\circ_i(T,P)$	5.70	
	$\Delta_f H^\circ$	----	Evaluate $\Delta_r h^\circ$ for reaction: $(1-y)Fe + y/2\ O_2 = Fe_{1-y}O$.
	$H^\circ_i(T)-H^\circ_i(Tr)$	5.71	Evaluate at T and Tr. Then take difference.
Gibbs energy	$g^\circ_i(T,P)$	5.65	
	$\Delta_f G^\circ$	----	Evaluate $\Delta_r g^\circ$ for reaction: $(1-y)Fe + y/2\ O_2 = Fe_{1-y}O$.
Gibbs energy function	$gef^\circ_i(T)$	7.44	Evaluate $h^\circ(Fe_{1-y}O)$ and $g^\circ(Fe_{1-y}O)$ as given above.
Empirical functions	r(T)	5.45	See also 7.49
	s(T)	5.45	See also 7.50
Log activity	log a(Fe)	5.57	
	log a(FeO)	5.61	
	log $a(O_2)$	5.44,5.45	See also 7.48, 7.49, 7.50.
	log $[a(CO_2)/a(CO)]$	5.78	
	log $[a(H_2O)/a(H_2)]$	5.78	Replace $g^\circ(CO_2)$ and $g^\circ(CO)$ by $g^\circ(H_2O)$ and $g^\circ(H_2)$, resp.
Composition	x, given y or y, given x	3.13	
	x, given log $a(O_2)$	----	= [log $a(O_2)$-r(T)]/s(T)
Volume	V	7.07	
Coefficient of volume expansion	α	5.15	No significant compositional dependence noted.
Coefficient of volume compression	β	5.19	No significant compositional dependence noted.

Table B.3 Continued Equations used to calculate thermodynamic properties of wustite, $Fe_{1-y}O$ or FeO_{1+x}, in standard conventions.

Calculations at the Iron-Wustite Boundary

Log activity	log a(Fe)	= 0.0	Iron is at unit activity.
	log a(FeO)	5.61	where $x=x_a$ and is evaluated from 5.48.
	log $a(O_2)$ = a(T) or a'(T)	5.46,5.45	See also 7.53 and 7.54.
Composition	x_a	5.48	
Volume	V	7.07	where y is evaluated by 5.48 and 3.13.
Coefficient of volume expansion	α	5.15	No significant compositional dependence noted.
Coefficient of volume compression	β	5.19	No significant compositional dependence noted.

Calculations at the Wustite-Magnetite Boundary

Log activity	log a(Fe)	5.57	where $x=x_b$ and is evaluated from 5.49.
	log a(FeO)	5.61	where $x=x_b$ and is evaluated from 5.49.
	log $a(O_2)$ = b(T)	5.47,5.45	See also 7.57.
Composition	x_b	5.49	
Volume	V	7.07	where y is evaluated by 5.49 and 3.13.
Coefficient of volume expansion	α	5.15	No significant compositional dependence noted.
Coefficient of volume compression	β	5.19	No significant compositional dependence noted.

Recommended Standard Electrochemical Potentials and Fugacities of Oxygen for the Solid Buffers and Thermodynamic Data in the Systems Iron-Silicon-Oxygen, Nickel-Oxygen, and Copper-Oxygen

Part 3
Legends for Figures

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Recommended fugacities and standard electrochemical potentials for O_2 in the buffer pairs from 200 to 1800 K were derived from critical reviews of experimental data and thermodynamic theory. Included are C_p°, H°(T)-H°(298), [G°(T) -H°(298)]/T, S°, $\Delta_f H^\circ$, $\Delta_f G^\circ$, V°, and the coefficients of volume expansion and of volume compression for the oxide phases.

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Figure 1.1. Example of the calculated electrochemical potential of O_2(ideal gas) for the solid chemical buffer assemblage quartz + fayalite + magnetite as published or cited since 1980:

square	Chou (1978)
triangle	Hewitt (1978)
plus	Schwab and Kuestner (1981)
circle	Myers and Eugster (1983)
diamond	O'Neill (1987)

Figure 3.1. Molar volume of quartz as a function of temperature. At 1 bar, alpha quartz is stable below and beta quartz is stable above 847 K. The line is a fit to the data. The data above 1400 K are contaminated by the presence of beta cristobalite. The sources of data are as follows:

circle	Ackermann and Sorrell (1974)
square	Jay (1933)
triangle	Berger and others (1966)

Figure 3.2. The molar volume of alpha quartz at ambient temperature as a function of pressure. The line is a fit to the data. The sources of data are as follows:

circle	Adams and others (1919)
square	d'Amour and others (1979)
triangle	Levin and others (1980)
diamond	Olinger and Halleck (1976)
inv tri	Vaidya and others (1973)

Figure 3.3. The molar volume of cristobalite at ambient pressure as a function of temperature. The break in the data at 543 K marks the alpha-beta inversion. The line is a fit to the data. The sources of data are as follows:

circle	Berger and others (1966)
square	Johnson and Andrews (1956)
triangle	Wright and Leadbetter (1975)

Figure 3.4. A portion of the phase diagram for the iron-oxygen system showing the phase relations for wustite as prepared by Darken and Gurry (1945, 1946). The symbol "●" represent experimental data. The symbol "+" represent estimations. The compositional limits of the wustite stability field below 1300 K was based on estimates.

Figure 5.1. Molar volume of bunsenite, NiO, at ambient pressure as a function of temperature. The line was calculated from the results of the optimization. The sources of data are as follows:

circle	Barrett and Evans (1964)
plus	Gillam and Holden (1953)
square	Bickelhaupt and others (1967)
triangle	Wisely (1962)
diamond	Melik-Davtyan and others (1966)
inv tri	Srivastava and others (1977)
"x"	Leipold and Niel~~s~~sen (1964)

Figure 5.2. Molar volume of bunsenite, NiO, at ambient temperature as a function of pressure. The line was calculated from the results of the optimization. The sources of data are as follows:

plus	Wakabayashi and others (1968)
diamond	Clendenen and Drickamer (1966)

Figure 5.3. Coefficient of volume expansion for fayalite, Fe_2SiO_4, at ambient pressure as measured by Suzuki and others (1981). The line is a fit to all the volume data for fayalite and shows the general form of the curve as a function of temperature. The measurements are in error because they show an anomalous increase in slope with increasing temperature whereas the data should be approaching a constant value as shown by the fitted curve.

Figure 5.4. Molar heat capacity at constant pressure for bunsenite, NiO, as a function of temperature. The cusp at 519 K is associated with the Neél transition. The line was calculated from the results of the optimization. The sources of data are as follows:

plus	King (1957)
square	Hemingway (1984)
diamond	Seltz and others (1940)

Figure 5.5. Detail of the heat capacity function near the Neél transition for bunsenite, NiO. At 519 K there is a nonsignificant break in the function of about 0.7 J/(mol K). Refer to the text for a discussion of the cause of the break in the fitted function.

Figure 5.6. Examples of the relation between log $a(O_2)$ and "x", the amount of excess oxygen in the wustite formula, FeO_{1+x}. The lines are calculated from this study. The sources of data are as follows:

circle	Bransky and Hed (1968)
square	Levin and Wagner (1966)
triangle	Gerdanian and Dodé (1965)
diamond	Marion (1955)

Figure 7.01. Molar volume for nickel, Ni, at ambient pressure as a function of temperature. The data were taken from Owen and Yates (1936). The line was fitted in this study. Refer to the text for a discussion of the anomaly at 631 K.

Figure 7.02. The ratio, (V-Vr)/Vr, as a function of temperature for nickel, Ni. The data were taken from the study by Nix and MacNair (1941) but only every fifth datum was plotted. The line is calculated from the fit from this study.

Figure 7.03. Molar volume of nickel, Ni, at ambient temperature as a function of pressure. The data were taken from the compilation by Birch (1966). The line was calculated from the results of the optimization.

Figure 7.04. Molar volume of bunsenite, NiO at ambient pressure as a function of temperature. The line was calculated from the results of the optimization. The sources of data are as follows:

circle	Barrett and Evans (1964)
plus	Gillam and Holden (1953)
square	Bickelhaupt and others (1967)
triangle	Wisely (1962)
diamond	Melik-Davtyan and others (1966)
inv tri	Srivastava and others (1977)
"x"	Leipold and Niel~~s~~sen (1964)

Figure 7.05. Molar volume of bunsenite, NiO, at ambient temperature as a function of pressure. The line was calculated from the results of the optimization. The sources of data are as follows:

plus	Wakabayashi and others (1968)
diamond	Clendenen and Drickamer (1966)

Figure 7.06. Molar volume of iron, Fe at ambient pressure as a function of temperature. The upper and lower lines are fits for the data for alpha and gamma iron, respectively. Refer to the text for a discussion of the data near 1042 K. On part a, the sources of data are as follows:

circle	Watanabe and others (1981)
plus	Skinner (1966)
square	Gorton and others (1965)
triangle	Robie and others (1979)
diamond	Basinski and others (1955)

On part b, the data were taken from Esser and Mueller (1933) and represent three different experimental runs.

Figure 7.07. The ratio (V-Vr)/Vr for iron, Fe, at ambient pressure as a function of temperature. The data were taken from Nix and MacNair (1941). Only every fifth value was plotted so that the location of the fitted curve could be seen.

Figure 7.08. Molar volume of iron, Fe, at ambient temperature as a function of pressure. Alpha iron is metastable and epsilon iron is stable above about 115 kbars. All data are for alpha iron. The line was a fit of the data from the following sources:

circle	Birch (1966)
plus	Clendenen and Drickamer (1964)
square	Jephcoat and others (1986)
triangle	Giles and others (1971)
diamond	Mao and others (1967)
inv tri	Wilburn and Bassett (1978)
"x"	Takahashi and others (1968)

Figure 7.09. Molar volume of wustite solid solution, $Fe_{1-y}O$ or FeO_{1+x} as a function of y, the iron deficit to the stoichiometric formula. The lines are a fit of the data which represent the volumes of quenched samples as supplied by the following authors: On part a,

circle	Hentschel (1970)
square	Levin and Wagner (1966)
triangle	Carel and Gavarri (1976), quenched from 1000°C
diamond	(same), quenched from 1200°C
inv tri	(same), quenched from 1340°C

On part b,

circle	Marion (1955)
square	Fujii and Meussner (1968)
triangle	Hazen (1981)
diamond	Yagi and others (1985)
inv tri	Will and others (1980)
"x"	Bonczar and Graham (1982)

Figure 7.10. Molar volume of wustite, $Fe_{1-y}O$ or FeO_{1+x}, at ambient pressure as a function of the iron deficit y. The data were taken from Touzelin (1974) and represent from bottom to top the isotherms at 1073 K, 1173 K, 1273 K, and 1348 K, respectively. The lines are fits calculated from equation 7.07. The data plotting on the ordinate at 0.0 are the molar volumes coexisting with alpha and gamma iron.

Figure 7.11. Molar volumes of wustite, $Fe_{1-y}O$ or FeO_{1+x}, at ambient temperature as a function of pressure. The lines were calculated from equation 7.07. The sources of data are as follows: On part a, all data were taken from Hazen (1981). The compositions are as follows:

circle	y = 0.100 moles
square	y = 0.070 moles
triangle	y = 0.053 moles
inv tri	y = 0.053 moles

On part b, the sources of data and compositions are as follows:

circle	Yagi and others (1985), y = 0.020 moles
square	Will and others (1980), y = 0.059 moles
triangle	Clendenen and Drickamer (1966), y = 0.067 moles
diamond	Mao and others (1969), y = 0.076 moles

On part c, the data were taken from Jeanloz and Sato-Sorenson (1986). For these data, y = 0.055 moles.
Refer to the text for a discussion of the data.

Figure 7.12. Molar volumes for hematite, Fe_2O_3, at ambient pressure as a function of temperature. The line was calculated from the results of the optimization. The data were taken from the following sources:

plus	Gordon and others (1965)
square	Willis and Rooksby (1952)
diamond	Robie and others (1979)
"x"	Neskovic (1984)

Figure 7.13. Molar volumes of hematite, Fe_2O_3, at ambient temperature as a function of pressure. The line was calculated from the results of the optimization. The data were taken from the following sources:

circle	Sato and Akimoto (1979)
plus	Finger and Hazen (1980)
square	Wilburn and others (1978)
diamond	Lewis and Drickamer (1966)

The data of Lewis and Drickamer (1966) do not represent measurements under a homogeneous pressure medium.

Figure 7.14. Molar volumes of fayalite, Fe_2SiO_4, as a function of temperature at ambient pressure. The line is a fit to the data. The data were taken from the following sources:

circle	Suwa (1974)
plus	Hazen (1977)
square	Suzuki and others (1981)
diamond	Schwab and Sohnlein (1977)
inv tri	Takei (1978)
"x"	Smyth (1975)

Figure 7.15. The apparent coefficient of volume expansion for fayalite, Fe_2SiO_4, as a function of temperature at ambient pressure. The data were taken from Rigby and others (1945) and represent mechanically measured changes in volume. Because of imperfections in such samples, the data are not equivalent to those data measured using X-ray techniques. The line was calculated from the results of the optimization.

Figure 7.16. Molar volume of fayalite, Fe_2SiO_4, as a function of pressure at ambient temperature. The line shows the fitted function. The data came from the following sources:

"x"	Yagi and others (1974)
circle	Yagi and others (1975)
plus	Hazen (1977)
triangle	Kudoh and Takeda (1986)

Figure 7.17. Molar volume of the spinel dimorph of fayalite, Fe_2SiO_4, at ambient pressure as a function of temperature. The line represents a linear fit of the data which were taken from the following sources:

circle	Mao and others (1969)
square	Marumo and others (1977)
triangle	Yamanaka (1986)

Figure 7.18. Molar volume of the spinel dimorph, Fe_2SiO_4, at ambient temperature as a function of pressure. The line was calculated from the results of the optimization taken from the following sources:

circle	Mao and others (1969)
square	Sato (1977)
diamond	Wilburn and Bassett (1978)

Figure 7.19. The Neél temperature as a function of pressure for magnetite, Fe_3O_4. The line was calculated from the results of the optimization taken from Samara and Giardini (1969).

Figure 7.20. The molar volume of magnetite, Fe_3O_4, at ambient pressure as a function of temperature. The line is a fit to the data taken from the following sources:

circle	Ellefson and others (1934)
plus	Sharma (1950)
square	Gorton and others (1965)
triangle	Nakagiri and others (1986)
diamond	Tombs and Rooksby (1951)
"x"	Yoshida and Iida (1979)

Refer to the text for a discussion of the data.

Figure 7.21. Molar volume of magnetite, Fe_3O_4 at ambient temperature as a function of pressure. The line is a fit of the data. The sources of data are as follows:

circle	Nakagiri and others (1986)
plus	Wilburn and Bassett (1977)
square	Finger and others (1986)
"x"	Mao and others (1974)

Figure 7.22. Molar heat capacity for tenorite, CuO, as a function of temperature. The line was calculated from the results of the optimization measured by Hu and Johnson (1953). The sources of data are as follows:

plus	Hu and Johnson (1943)
"x"	Millar (1929)
diamond	Clusius and Harteck (1928)

The data near the Neèl temperature poorly define the function. Additional experiments would be useful.

Figure 7.23. Heat content data for tenorite, CuO, above room temperature. The plotted data were taken from Mah and others (1967). The line was calculated from the results of the optimization.

Figure 7.24. Molar heat capacities for cuprite, Cu_2O, as a function of temperature. The line was derived from the optimization. The sources of data are as follows:

plus	Mah and others (1967)
"x"	Millar (1929)
diamond	Hu and Johnson (1951)

Figure 7.25. Molar heat contents for cuprite, Cu_2O, to 1600 K. The melting temperature is 1516.7 K. The line was obtained from the optimization. The plotted data were taken from Mah and others (1967).

Figure 7.26. Molar heat capacity at constant pressure for bunsenite, NiO, as a function of temperature. The cusp at 519 K is associated with the Neèl transition. The line was calculated from the results of the optimization. The sources of data are as follows:

plus	King (1957)
square	Hemingway (1984)
diamond	Seltz and others (1940)

Figure 7.27. Molar heat content of bunsenite, NiO, as a function of temperature. The line was obtained from the optimization. The sources of data are as follows:

plus	King and Cristensen (1958)
diamond	Tomlinson and others (1955)

The data of Tomlinson and others have been corrected to a reference temperature of 298.15 K for plotting purposes.

Figure 7.28. Molar heat capacity at constant pressure for wustite, $Fe_{0.947}O$, as a function of temperature. The line is a result of the optimization. The sources of data are as follows:

circle	Millar (1929)
plus	Todd and Bonnickson (1951)

The measurements by Millar (1929) were given zero weight during the optimization.

Figure 7.29. Molar heat contents for wustite, $Fe_{0.947}O$, as a function of temperature. The data were taken from Coughlin and others (1951). The line is the result of the optimization.

Figure 7.30. Molar heat contents for wustites of different compositions. The temperature interval was between 1179 and 299 K. The line was calculated from the results of the optimization. The data shown as "+" were taken from the study by Rogez and others (1982). The datum shown as "o" was interpolated from the study by Coughlin and others (1951). The optimization has shown that the data by Rogez and others are too low by about 5 percent. However the trend with composition is compatible with that derived from the optimization.

Figure 7.31. Molar heat capacity at constant pressure for hematite, Fe_2O_3, as a function of temperature. The line is the result of the optimization. The data were taken from the following sources:

circle	Parks and Kelley (1926)
plus	Grønvold and Samuelsen (1975)
square	Krupka (1974)
"x"	Grønvold and Westrum (1959)

Figure 7.32. Molar heat contents for hematite, Fe_2O_3, as a function of temperature. The line was the result of the optimization. The sources of data are as follows:

circle	Roth and Bertram (1929)
plus	Esser and others (1933)
square	Reznitsky and Filippova (1972)
diamond	Coughlin and others (1951)

Figure 7.33. Molar heat capacity at constant pressure for fayalite, Fe_2SiO_4, as a function of temperature. The line was calculated from the optimization results. The sources of data are as follows:

circle	Watanabe (1982)
plus	Robie and others (1982)
"x"	Osako (1980)
diamond	Kelley (1941)

Figure 7.34. Molar heat content for fayalite and the liquid Fe_2SiO_4 as a function of temperature. The lines were calculated from the results of the optimization. The metastable congruent melting temperature is taken as 1490 K. The calculated heat contents of the liquid have been modified to reflect the heat of fusion reported by Stebbins and Carmichael (1984). The sources of data are as follows:

circle	Roth and Bertram (1929)
plus	Orr (1953)

Figure 7.35. Molar heat capacity at constant pressure for the spinel dimorph, Fe_2SiO_4, as a function of temperature. The line was obtained from the optimization. The sources of data are as follows:

circle	Osako (1980)
plus	Watanabe (1982)

Figure 7.36. Molar heat content for the spinel dimorph, Fe_2SiO_4, as a function of temperature. The line was calculated from the results of the optimization. The data were taken from Agoshkov (1985).

Figure 7.37. Molar heat capacity at constant pressure for magnetite, Fe_3O_4, as a function of temperature. The line was calculated from the results of the optimization. The sources of data are as follows:

plus	Grønvold and Sveen (1974)
square	Bartel and Westrum (1975)
triangle	Parks and Kelley (1926)
diamond	Millar (1929)
"x"	Westrum and Grønvold (1969)

Figure 7.38. Molar heat content for magnetite, Fe_3O_4, as a function of temperature. The line was calculated from the optimization. The sources of data is as follows:

circle	Roth and Bertram (1929)
plus	Esser and others (1933)
diamond	Coughlin and others (1951)

Figure 7.39. A graphic representation of the reaction network solved during the optimization. The elipses represent the properties of the chemical components as labeled. The straight lines connecting the elipses represent reactions that were balanced by O_2(ideal gas). The curved lines represent "cross-reactions" among the phases. Refer to the text for more detail.

Figure 7.40. Plot of the third-law enthalpy of reaction at 298.15 K as a function of temperature for the equilibria between wustite solid solution and the gases CO and CO_2., The line was obtained from the optimization. The sources of data are as follows: For part a,

circle	Ackermann and Sanford (1966)
plus	Bransky and Hed (1968)
square	Darken and Gurry (1945)
triangle	Gavarri and others (1979)
diamond	Gerdanian and Dodé (1965)
inv tri	Levin and Wagner (1966)

For part b,

circle	Swaroop and Wagner (1967)
plus	Touzelin (1974)
square	Vallet and Raccah (1965)

Figure 7.41. Plot of the third-law enthalpy of reaction at 298.15 K as a function of composition for the equilibria between wustite solid solution and the gases CO and CO_2. The line was obtained from the optimization. The sources of data are as follows: For part a,

circle	Ackermann and Sanford (1966)
plus	Bransky and Hed (1968)
square	Darken and Gurry (1945)
triangle	Gavarri and others (1979)
diamond	Gerdanian and Dodé (1965)
inv tri	Levin and Wagner (1966)

For part b,

circle	Swaroop and Wagner (1967)
plus	Touzelin (1974)
square	Vallet and Raccah (1965)

Figure 7.42. Plot of the third-law enthalpy of reaction at 298.15 K as a function of temperature for the equilibria between wustite solid solution and the gases H_2 and H_2O. The line was obtained from the optimization. The sources of data are as follows: For part a,

square	Lohberg and Stannek (1975)
triangle	Marion (1955)
diamond	Riecke and Bohnenkamp (1969)

The data by Marion (1955) were given a low weight because they might be in error due to chemical disequilbirum caused by Soret phenomenon.

Figure 7.43. Plot of the third-law enthalpy of reaction at 298.15 K as a function of composition for the equilibria between wustite solid solution and the gases H_2 and H_2O. The line was obtained from the optimization. The sources of data are as follows:

square	Lohberg and Stannek (1975)
triangle	Marion (1955)
diamond	Riecke and Bohnenkamp (1969)

The data by Marion (1955) were given a low weight because they might be in error due to chemical disequilbrium caused by Soret phenomenon.

Figure 7.44. Pressure-temperature plot showing the stability fields of the three polymorphs of Fe_2SiO_4. The lines were calculated from the results of the optimization. The invariant point is near 1823 K (1550°C) and 66 kbars. The sources of data are as follows:

circle	Akimoto and others (1967)
plus	Akimoto and others (1977)
square	Akimoto and Yagi (1986)
triangle	Hsu (1967)
diamond	Lindsley (1967)
inv tri	Ohtani and others (1979)

Figure 7.45. Contours of temperature as a function of log $a(O_2)$ and composition.

Figure 7.46. Contours of log a(Fe) as a function of temperature from 800 to 1700 K. The contour interval is 0.01 in y. The stability field of wustite lies between the horizontal line at log a(Fe) = 0 and the lower line that crosses the contours with a negative slope. The first line is the iron-wustite boundary and the second is the wustite-magnetite boundary.

Figure 7.47. Contours of log a(FeO) as a function of temperature from 800 to 1700 K. The contour interval is 0.01 in y. The stability field lies between the upper and lower lines that cross the contours. The upper line is the iron-wustite boundary and the lower line is the wustite-magnetite boundary.

Figure 7.48. Plot of available data for the composition of the wustite phase coexisting with metallic iron. The stability field was calculated from the results of the optimization. The data for the liquid field was taken from the experimental study by Darken and Gurry (1945). The plotted data are taken from the following sources: For part a,

circle	Ackermann and Sanford (1966)
plus	Asao and others (1970)
square	Barbi (1964a)
triangle	Campserveux and others (1970)
diamond	Cirilli and others (1970)
"x"	Darken and Gurry (1945)

For part b,

For part b,

circle	Engell (1957)
plus	Fujii and Meussner (1968)
inv tri	Hoffmann (1959)
square	Lykasov and others (1969)
triangle	Marion (1955)
diamond	Marucco and others (1970)
"x"	Schenck and others (1927)

For part c,

circle	Swaroop and Wagner (1967)
plus	Takayama and Kimizuka (1980)
square	Touzelin (1974)
triangle	Vallet and Raccah (1965)

Figure 7.49. Plot of the data measured by Ariya and Yakovleva (1970) and the calculated contours for each experimental composition. Only the data for the comparison of the wustite-magnetite boundary against the reference iron-wustite boundary is in agreement with the results from the optimization. The other data is displaced to lower oxygen contents from the calculated values. This is consistent with loss of oxygen from the wustite sample to the iron-wustite reference sample where the oxygen would convert iron to more wustite.

Figure 7.50. Plot of available data for the composition of the wustite phase coexisting with magnetite. The stability field was calculated from the results of the optimization. The data for the liquid field was taken from the experimental study by Darken and Gurry (1945). The plotted data are taken from the following sources:

For part a,

circle	Ackermann and Sanford (1966)
plus	Ariya and Yakovleva (1970)
square	Asao and others (1970)
triangle	Barbi (1964a)
diamond	Campserveux and others (1970)
"x"	Cirilli and others (1970)

For part b,

circle	Darken and Gurry (1945)
plus	Engell (1957)
inv tri	Fischer and Hoffmann (1958)
square	Fujii and Meussner (1968)
triangle	Giddings (1972)
diamond	Lykasov and others (1969)
"x"	Marion (1955)

For part c,

circle	Marucco and others (1970)
plus	Schenck and others (1927)
square	Takayama and Kimizuka (1980)
triangle	Touzelin (1974)
diamond	Vallet and Raccah (1965)

Figure 7.51. Compositions differences, x_b-x_a, measured for the wustite stability field as measured by coulometric titration. The line was calculated from the optimization. The sources of data are as follows:

circle	Giddings (1972)
plus	Sockel and Schmalzried (1968)

Figure 10.1. Plot of the electrochemical potentials for the solid buffers relative to 1 bar $O_2(g)$ from 200 to 1800 K.

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Figure A.01. Plot of log K for the reaction "$2\ Cu + 0.5\ O_2 = Cu_2O$" as a function of reciprocal temperature. The line was obtained from the optimization. The sources of data are as follows For part a,

circle	Fischer and Pateisky (1970)
plus	Holmes and others (1986)
square	Kemora and others (1979)
triangle	Kodera and others (1983)
diamond	Matsushita and Goto (1963)
"x"	Peters (1983)

For part b,

circle	Rizzo and others (1967)
plus	Slobodyanyuk and others (1973)
square	Treadwell (1916)
triangle	Tretyakov and Schmalzried (1965)

Figure A.02. Plot of $\Delta_r H^\circ(298)$ for the reaction "$2\ Cu + 0.5\ O_2 = Cu_2O$" as a function of temperature. The line was obtained from the optimization. The sources of data are as follows: For part a,

circle	Fischer and Pateisky (1970)
plus	Holmes and others (1986)
square	Kemora and others (1979)
triangle	Kodera and others (1983)
diamond	Matsushita and Goto (1963)
"x"	Peters (1983)

For part b,

circle	Rizzo and others (1967)
plus	Slobodyanyuk and others (1973)
square	Treadwell (1916)
triangle	Tretyakov and Schmalzried (1965)

Figure A.03. Plot of log K for the reaction "$Cu_2O + CO = 2\ Cu + CO_2$" as a function of reciprocal temperature. The line was obtained from the optimization. The data were taken from Peters and Mann (1958).

Figure A.04. Plot of $\Delta_r H^\circ(298)$ for the reaction "$Cu_2O + CO = 2\ Cu + CO_2$" as a function of temperature. The line was obtained from the optimization. The data were taken from Peters and Mann (1958).

Figure A.05. Plot of log K for the reaction "$2\ Cu + O_2 = 2\ CuO$" as a function of reciprocal temperature. The line was obtained from the optimization. The data were taken from Matsushita and Goto (1963).

Figure A.06. Plot of $\Delta_r H^\circ(298)$ for the reaction "$2\ Cu + O_2 = 2\ CuO$" as a function of temperature. The line was obtained from the optimization. The data were taken from Matsushita and Goto (1963).

Figure A.07. Plot of log K for the reaction " $Cu_2O + 0.5\ O_2 = 2\ CuO$" as a function of reciprocal temperature. The line was obtained from the optimization. The data were taken from the following sources: For part a,

circle	Hochgeschwender and others (1967)
plus	Kodera and others (1968)
square	Landolt and Muan (1969)
triangle	Norton (1955)
diamond	Peters (1983)
inv tri	Rog (1976)

For part b,

circle	Slobodyanyuk and others (1973)
plus	Treadwell (1916)
square	Vasileva and others (1975)

Figure A.08. Plot of $\Delta_r H^\circ(298)$ for the reaction " $Cu_2O + 0.5\ O_2 = 2\ CuO$" as a function of temperature. The line was obtained from the optimization. The data were taken from the following sources: For part a,

circle	Hochgeschwender and others (1967)
plus	Kodera and others (1968)
square	Landolt and Muan (1969)
triangle	Norton (1955)
diamond	Peters (1983)
inv tri	Rog (1976)

For part b,

circle	Slobodyanyuk and others (1973)
plus	Treadwell (1916)
square	Vasileva and others (1975)

Figure A.09. Plot of log K for the reaction "$Ni + 0.5\ O_2 = NiO$" as a function of reciprocal temperature. The line was obtained from the optimization. The data were taken from the following sources: For part a,

circle	Barbi (1964a,b)
plus	Berglund (1976)
square	Charette (1967)
triangle	Comert and Pratt (1984)
diamond	Fischer and Pateisky (1970)
inv tri	Grimley and others (1961)

For part b,

circle	Holmes and others (1986)
plus	Huebner and Sato (1970)
square	Iwase and others (1975, 1978)

For part c,

circle	Kazenas and others (1969)

plus	Kemori and others (1979)
square	Kodera and others (1968)
triangle	Meier and Rapp (1971)
diamond	Moriyama and others (1969)
inv tri	Moser and others (1975)

For part d,

circle	Myers and Gunther (1979)
plus	Oishi and others (1972)
square	Ray and others (1974)
triangle	Rog (1976)
diamond	Saito and others (1972, 1975)
inv tri	Schwab and Kuestner (1981)

For part e,

circle	Sockel and Schmalzried (1968)
plus	Taylor and Schmalzried (1964)
square	Tran and Brungs (1980)
triangle	Treadwell (1916)
diamond	Tretyakov and Schmalzried (1965)
inv tri	Trumm (1971)

Figure A.10. Plot of $\Delta_rH°(298)$ for the reaction "$Ni + 0.5\ O_2 = NiO$" as a function of temperature. The line was obtained from the optimization. The data were taken from the following sources:

For part a,

circle	Barbi (1964a,b)
plus	Berglund (1976)
square	Charette (1967)
triangle	Comert and Pratt (1984)
diamond	Fischer and Pateisky (1970)
inv tri	Grimley and others (1961)

For part b,

circle	Holmes and others (1986)
plus	Huebner and Sato (1970)
square	Iwase and others (1975, 1978)

For part c,

circle	Kazenas and others (1969)
plus	Kemori and others (1979)
square	Kodera and others (1968)
triangle	Meier and Rapp (1971)
diamond	Moriyama and others (1969)
inv tri	Moser and others (1975)

For part d,

circle	Myers and Gunther (1979)
plus	Oishi and others (1972)
square	Ray and others (1974)
triangle	Rog (1976)
diamond	Saito and others (1972, 1975)
inv tri	Schwab and Kuestner (1981)

For part e,

circle	Sockel and Schmalzried (1968)
plus	Taylor and Schmalzried (1964)

square	Tran and Brungs (1980)
triangle	Treadwell (1916)
diamond	Tretyakov and Schmalzried (1965)
inv tri	Trumm (1971)

Figure A.11. Plot of log K for the reaction "$NiO + CO = Ni + CO_2$" as a function of reciprocal temperature. The line was obtained from the optimization. The sources of data are as follows:

circle	Antill and Warburton (1967)
plus	Fricke and Weitbrecht (1942)
square	Klinedinst and ~~Stepheson~~ (1972) Stevenson
triangle	Navrotsky and Muan (1970)
diamond	Peters and Muan (1958)
inv tri	Tomlinson and Young (1964)
"x"	Watanabe (1933)

Figure A.12. Plot of $\Delta_r H^\circ(298)$ for the reaction "$NiO + CO = Ni + CO_2$" as a function of temperature. The line was obtained from the optimization. The sources of data are as follows:

circle	Antill and Warburton (1967)
plus	Fricke and Weitbrecht (1942)
square	Klinedinst and Stepheson (1972)
triangle	Navrotsky and Muan (1970)
diamond	Peters and Muan (1958)
inv tri	Tomlinson and Young (1964)
"x"	Watanabe (1933)

Figure A.13. Plot of log K for the reaction "$NiO + H_2 = Ni + H_2O$" as a function of reciprocal temperature. The lines were obtained from the optimization. The upper line represents the equilibrium at 2 kbars, the lower line at 1 atm. The data of Gunther and others (1979) were measured at 2 kbars, the others at 1 atm nominal. The sources of data are as follows:

plus	Gunther and others (1979)
square	Pease and Cook (1926)
triangle	Rau and Guedes de Carvalho (1973)

The data of Babushkin and others (1971) did not plot on the figure and are in error.

Figure A.14. Plot of $\Delta_r H^\circ(298)$ for the reaction "$NiO + H_2 = Ni + H_2O$" as a function of temperature. The line was calculated from the optimization. The sources of data are as follows:

plus	Gunther and others (1979)
square	Pease and Cook (1926)
triangle	Rau and Guedes de Carvalho (1973)

Figure A.15. Plot of E for the reaction "$Cu_2O + Ni + 2\ Cu + NiO$" as a function of temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Bidwell and Speiser (1963)
plus	Bonnet and Perrin (1978)
square	Bugden (1967)
triangle	Charette (1967)
diamond	Moriyama and others (1969)
inv tri	Moser and others (1975)

For part b,

circle	Pyun and Mueller (1977)
plus	Ramakrishnan and others (1975)
square	Rizzo and others (1967)
triangle	Sebkova and Baranek (1975)
diamond	Sellars and Maak (1966)
inv tri	Shaiu and others (1977)

For part c,

circle	Steele and Alcock (1965)
plus	Trumm (1971)
square	Vasileva and others (1975)

Figure A.16. Plot of $\Delta_r H°(298)$ for the reaction "$Cu_2O + Ni + 2\ Cu + NiO$" as a function of temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Bidwell and Speiser (1963)
plus	Bonnet and Perrin (1978)
square	Bugden (1967)
triangle	Charette (1967)
diamond	Moriyama and others (1969)
inv tri	Moser and others (1975)

For part b,

circle	Pyun and Mueller (1977)
plus	Ramakrishnan and others (1975)
square	Rizzo and others (1967)
triangle	Sebkova and Baranek (1975)
diamond	Sellars and Maak (1966)
inv tri	Shaiu and others (1977)

For part c,

circle	Steele and Alcock (1965)
plus	Trumm (1971)
square	Vasileva and others (1975)

Figure A.17. Plot of E for the reaction "2 CuO + Ni = Cu_2O + NiO" as a function of temperature. The line was calculated from the optimization. The data were taken from Charette (1967).

Figure A.18. Plot of $\Delta_r H^\circ(298)$ for the reaction "2 CuO + Ni = Cu_2O + NiO" as a function of temperature. The line was calculated from the optimization. The data were taken from Charette (1967).

Figure A.19. Comparison of the calculated intercept (line) with values derived from measurements on isotherms from the following studies: For part a,

circle	Ackermann and Sanford (1966)
plus	Ariya and others (1954)
square	Barbero and others (1981)
triangle	Bransky and Hed (1968)
diamond	Darken and Gurry (1945)
inv tri	Gerdanian and Dodé (1965)

For part b,

circle	Giddings (1972)
plus	Hauffe and Pfeiffer (1953)
square	Himmel and others (1953)
triangle	Janowski and others (1973)
diamond	Levin and Wagner (1966)
inv tri	Lohberg and Stannek (1975)

For part c,

circle	Marion (1955)
plus	Myers and Eugster (1983)
square	Riecke and Böhnenkamp (1969)
triangle	Rizzo and Smith (1968)
diamond	Smyth (1961)
inv tri	Swaroop and Wagner (1967)

For part d,

circle	Touzelin (1974)
plus	Vallet and Raccah (1965)
square	Gavarri and others (1979)
triangle	Picard and Dodé (1970)

Figure A.20. Comparison of the calculated slope (line) with values derived from measurements on isotherms from the following studies: For part a,

circle	Ackermann and Sanford (1966)
plus	Ariya and others (1954)
square	Barbero and others (1981)
triangle	Bransky and Hed (1968)
diamond	Darken and Gurry (1945)
inv tri	Gerdanian and Dodé (1965)

For part b,

circle	Giddings (1972)
plus	Hauffe and Pfeiffer (1953)
square	Himmel and others (1953)
triangle	Janowski and others (1973)

diamond	Levin and Wagner (1966)
inv tri	Lohberg and Stannek (1975)

For part c,

circle	Marion (1955)
plus	Myers and Eugster (1983)
square	Riecke and Bohnenkamp (1969)
triangle	Rizzo and Smith (1968)
diamond	Smyth (1961)
inv tri	Swaroop and Wagner (1967)

For part d,

circle	Touzelin (1974)
plus	Vallet and Raccah (1965)
square	Gavarri and others (1979)
triangle	Picard and Dodé (1970)

Figure A.21. Plots of $\Delta_r H°(298)$ for the reaction "2 FeO(wus,sln) = 2 Fe(wus,sln) + O_2" as a function of the excess oxygen in the formula FeO_{1+x}. The sources of data are given on each graph. The symbol "o" locates data not used in the optimization, the symbol "●" locate~~d~~s data used in the optimization.

Figure A.22. Plot of log $a(O_2)$ for the reaction "2 FeO(wus,sln) = 2 Fe + O_2" at the iron-wustite boundary as a function of reciprocal temperature. The line was obtained from the optimization. The sources of data are as follows: For part a,

circle	Barbero and others (1981)
plus	Fischer and Pateisky (1970)
square	Hahn and Muan (1962)
triangle	Holmes and others (1986)
diamond	Jacobsson and Rosén (1981)
inv tri	Mallika and others (1986)

For part b,

circle	Matsushita and Goto (1963)
plus	Myers and Eugster (1983)
square	Myers and Gunther (1979)
triangle	Rog (1976)
diamond	Schwab and Kuestner (1981)
inv tri	Sockel and Schmalzried (1968)

For part c,

plus	Rizzo (1968)

For part d,

circle	Sugimoto and others (1980)
plus	Takayama and Kimizuka (1980)
square	Taylor and Schmalzried (1964)
triangle	Treadwell (1916)
diamond	Tretyakov and Schmalzried (1965)
inv tri	Vallet (1965)

Figure A.23. Plot of $\Delta_r H°(298)$ for the reaction "2 FeO(wus,sln) = 2 Fe + O_2" at the iron-wustite boundary as a function of temperature. The line was obtained from the optimization. The sources of data are as follows: For part a,

circle	Barbero and others (1981)
plus	Fischer and Pateisky (1970)
square	Hahn and Muan (1962)
triangle	Holmes and others (1986)
diamond	Jacobsson and Rosèn (1981)
inv tri	Mallika and others (1986)

For part b,

circle	Matsushita and Goto (1963)
plus	Myers and Eugster (1983)
square	Myers and Gunther (1979)
triangle	Rog (1976)
diamond	Schwab and Kuestner (1981)
inv tri	Sockel and Schmalzried (1968)

For part c,

plus	Rizzo (1968)

For part d,

circle	Sugimoto and others (1980)
plus	Takayama and Kimizuka (1980)
square	Taylor and Schmalzried (1964)
triangle	Treadwell (1916)
diamond	Tretyakov and Schmalzried (1965)
inv tri	Vallet (1965)

Figure A.24. Plot of log [$a(CO_2)/a(CO)$] for the reaction "FeO(wus,sln) + CO = Fe + CO_2" at the iron-wustite boundary as a function of reciprocal temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Ariya and others (1954)
plus	Chaudron (1921)
square	Darken and Gurry (1945)
triangle	Fakhoury and Rosenqvist (1976)
diamond	Garran (1928)
inv tri	Golubenko and Rez~~h~~ukhina (1964)

For part b,

circle	Kiukkola and Wagner (1957)
plus	Kondakov and Wan (1958)
square	Marion (1955)
triangle	Marucco and others (1970)
diamond	Matsubara (1922)
inv tri	Peters and Mann (1958)

For part c,

circle	Schenck and others (1927)
plus	Schenck and others (1929)
square	Schwerdtfeger and Muan (1966)
triangle	Touzelin (1974)
diamond	Vallet and Raccah (1965)
inv tri	Schwerdtfeger and Muan (1967)

Figure A.25. Plot of $\Delta_r H^\circ(298)$ for the reaction "$FeO(wus,sln) + CO = Fe + CO_2$" at the iron-wustite boundary as a function of temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Ariya and others (1954)
plus	Chaudron (1921)
square	Darken and Gurry (1945)
triangle	Fakhoury and Rosenqvist (1976)
diamond	Garran (1928)
inv tri	Golubenko and Rez~~n~~ukhina (1964)

For part b,

circle	Kiukkola and Wagner (1957)
plus	Kondakov and Wan (1958)
square	Marion (1955)
triangle	Marucco and others (1970)
diamond	Matsubara (1922)
inv tri	Peters and Mann (1958)

For part c,

circle	Schenck and others (1927)
plus	Schenck and others (1929)
square	Schwerdtfeger and Muan (1966)
triangle	Touzelin (1974)
diamond	Vallet and Raccah (1965)
inv tri	Schwerdtfeger and Muan (1967)

Figure A.26. Plot of log $[a(H_2O)/a(H_2)]$ for the reaction "$FeO(wus,sln) + H_2 = Fe + H_2O$" at the iron-wustite boundary as a function of reciprocal temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Britzke and others (1934)
plus	Chaudron (1921)
square	Chipman and Marshall (1940)
triangle	Eastman and Evans (1924)
diamond	Edmiston and Grace (1966)
inv tri	Emmett and Shultz (1930)

For part b,

circle	Emmett and Shultz (1933)
plus	von Goldbeck (1949)
square	Jominy and Murphy (1931)
triangle	Marion (1955)
diamond	Rau (1972)
inv tri	Schreiner and Grimes (1920)

For part c,

circle	Viktorovich and others (1972)
plus	Woehler and Balz (1921)
square	Woehler and Gunther (1923)

Figure A.27. Plot of $\Delta_r H^\circ(298)$ for the reaction "$FeO(wus,sln) + H_2 = Fe + H_2O$" at the iron-wustite boundary as a function of temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Britzke and others (1934)
plus	Chaudron (1921)
square	Chipman and Marshall (1940)
triangle	Eastman and Evans (1924)
diamond	Edmiston and Grace (1966)
inv tri	Emmett and Shultz (1930)

For part b,

circle	Emmett and Shultz (1933)
plus	von Goldbeck (1949)
square	Jominy and Murphy (1931)
triangle	Marion (1955)
diamond	Rau (1972)
inv tri	Schreiner and Grimes (1920)

For part c,

circle	Viktorovich and others (1972)
plus	Woehler and Balz (1921)
square	Woehler and Gunther (1923)

Figure A.28. Plot of E for the reaction "$FeO(wus,sln) + 2\ Cu = Fe + Cu_2O$" as a function of temperature. The reaction is the potential difference between the iron-wustite buffer and the copper-cuprite buffer. The line was calculated from the optimization. The sources of data are as follows:

circle	Kiukkola and Wagner (1957)
plus	Steele and Alcock (1965)

Figure A.29. Plot of $\Delta_r H^\circ(298)$ for the reaction "$FeO(wus,sln) + 2\ Cu = Fe + Cu_2O$" as a function of temperature. The reaction is the potential difference between the iron-wustite buffer and the copper-cuprite buffer. The line was calculated from the optimization. The sources of data are as follows:

circle	Kiukkola and Wagner (1957)
plus	Steele and Alcock (1965)

Figure A.30. Plot of E for the reaction "$FeO(wus,sln) + Ni = Fe + NiO$" as a function of temperature. The reaction is the potential difference between the iron-wustite and the nickel-bunsenite buffers. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Asao and others (1970)
plus	Bonnet and Perrin (1978)
square	Catlow and others (1967)
triangle	Charette (1977)
diamond	Davies and Smeltzer (1972)
inv tri	Hoch and others (1962)

For part b,

circle	Jacobsson and Rosén (1981)

plus	Kiukkola and Wagner (1957)
square	Levitsky and others (1965)
triangle	Moriyama and others (1969)
diamond	Pyun and Mueller (1969)
inv tri	Ramakrishnan and others (1975)

For part c,

circle	Rapp (1963)
plus	Roedder and Smeltzer (1964)
square	Saito and others (1972, 1974)
triangle	Sjoeden and others (1986)
diamond	Sreedharan and others (1977)
inv tri	Steele and Alcock (1965)
"x"	Trumm (1971)

Figure A.31. Plot of $\Delta_r H^\circ(298)$ for the reaction "FeO(wus,sln) + Ni = Fe + NiO" as a function of temperature. The reaction is the potential difference between the iron-wustite and the nickel-bunsenite buffers. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Asao and others (1970)
plus	Bonnet and Perrin (1978)
square	Catlow and others (1967)
triangle	Charette (1977)
diamond	Davies and Smeltzer (1972)
inv tri	Hoch and others (1962)

For part b,

circle	Jacobsson and Rosén (1981)
plus	Kiukkola and Wagner (1957)
square	Levitsky and others (1965)
triangle	Moriyama and others (1969)
diamond	Pyun and Mueller (1969)
inv tri	Ramakrishnan and others (1975)

For part c,

circle	Rapp (1963)
plus	Roedder and Smeltzer (1964)
square	Saito and others (1972, 1974)
triangle	Sjoeden and others (1986)
diamond	Sreedharan and others (1977)
inv tri	Steele and Alcock (1965)
"x"	Trumm (1971)

Figure A.32. Plot of log K for the reaction "3 Fe + 2 O_2 = Fe_3O_4" as a function of reciprocal temperature. The line was calculated from the optimization. The sources of data are as follows:

circle	Barbi (1964a,b)
plus	Mallika and others (1986)
square	Matsushita and Goto (1963)
triangle	Stofko (1974)
diamond	Sugimoto and others (1980)

Figure A.33. Plot of $\Delta_r H^\circ(298)$ for the reaction "3 Fe + 2 O_2 = Fe_3O_4" as a function of temperature. The line was calculated from the optimization. The sources of data are as follows:

circle	Barbi (1964a,b)
plus	Mallika and others (1986)
square	Matsushita and Goto (1963)
triangle	Stofko (1974)
diamond	Sugimoto and others (1980)

Figure A.34. Plot of log K for the reaction "0.25 Fe_3O_4 + CO = 0.75 Fe + CO_2" as a function of reciprocal temperature. The line was calculated from the optimization. The data were taken from Marion (1955).

Figure A.35. Plot of $\Delta_r H^\circ(298)$ for the reaction "0.25 Fe_3O_4 + CO = 0.75 Fe + CO_2" as a function of temperature. The line was calculated from the optimization. The data were taken from Marion (1955).

Figure A.36. Plot of log K for the reaction "0.25 Fe_3O_4 + H_2 = 0.75 Fe + H_2O" as a function of reciprocal temperature. The line was calculated from the optimization. The sources of data are as follows:

circle	Chaudron (1921)
plus	Emmett and Shultz (1933)
square	Fricke and others (1941)
triangle	Marion (1955)
diamond	Rau (1972)
inv tri	Woehler and Gunther (1923)

Figure A.37. Plot of $\Delta_r H^\circ(298)$ for the reaction "0.25 Fe_3O_4 + H_2 = 0.75 Fe + H_2O" as a function of temperature. The line was calculated from the optimization. The sources of data are as follows:

circle	Chaudron (1921)
plus	Emmett and Shultz (1933)
square	Fricke and others (1941)
triangle	Marion (1955)
diamond	Rau (1972)
inv tri	Woehler and Gunther (1923)

Figure A.38. Plot of log $a(O_2)$ for the reaction "2 Fe_3O_4 = 6 FeO(wus,sln) + O_2" at the wustite-magnetite boundary as a function of reciprocal temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Barbero and others (1981)
plus	Carel (1971)
square	Chizhikov and others (1969)
triangle	Chizhikov and others (1971)
diamond	Gordeev (1966)
inv tri	Myers and Eugster (1983)

For part b,

plus	Rizzo (1968)

For part c,

circle	Petric and others (1981)
plus	Schwab and Kuestner (1981)
square	Shchedrin and others (1978)
triangle	Snethlage and Klemm (1975)
diamond	Snethlage and Schrocke (1976)
inv tri	Sockel and Schmalzried (1968)

For part d,

circle	Takayama and Kimizuka (1980)
plus	Treadwell (1916)
square	Vallet (1965)

Figure A.39. Plot of $\Delta_r H^\circ(298)$ for the reaction "2 Fe_3O_4 = 6 FeO(wus,sln) + O_2" at the wustite-magnetite boundary as a function of temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Barbero and others (1981)
plus	Carel (1971)
square	Chizhikov and others (1969)
triangle	Chizhikov and others (1971)
diamond	Gordeev (1966)
inv tri	Myers and Eugster (1983)

For part b,

plus	Rizzo (1968)

For part c,

circle	Petric and others (1981)
plus	Schwab and Kuestner (1981)
square	Shchedrin and others (1978)
triangle	Snethlage and Klemm (1975)
diamond	Snethlage and Schrocke (1976)
inv tri	Sockel and Schmalzried (1968)

For part d,

circle	Takayama and Kimizuka (1980)
plus	Treadwell (1916)
square	Vallet (1965)

Figure A.40. Plot of E for the reaction "Fe_3O_4 + Fe = 4 FeO(wus,sln)" as a function of temperature. The potentials represent the difference between the iron-wustite and the wustite-magnetite buffer assemblages. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Ariya and Yakovleva (1970)
plus	Barbi (1964a,b)
square	Birks (1966)
triangle	Eremenko and Filippov (1967)
diamond	Gordeev and Tretyakov (1963)
inv tri	Hoch and others (1962)

For part b,

circle	Jacobsson (1985)
plus	Kiukkola and Wagner (1957)
square	Levitsky and others (1965)

triangle	Moriyama and others (1969)
diamond	Roeder and Smeltzer (1964)
inv tri	Trumm (1971)

Figure A.41. Plot of $\Delta_{r}H^{\circ}(298)$ for the reaction "$Fe_3O_4 + Fe = 4\ FeO$(wus,sln)" as a function of temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Ariya and Yakovleva (1970)
plus	Barbi (1964a,b)
square	Birks (1966)
triangle	Eremenko and Filippov (1967)
diamond	Gordeev and Tretyakov (1963)
inv tri	Hoch and others (1962)

For part b,

circle	Jacobsson (1985)
plus	Kiukkola and Wagner (1957)
square	Levitsky and others (1965)
triangle	Moriyama and others (1969)
diamond	Roeder and Smeltzer (1964)
inv tri	Trumm (1971)

Figure A.42. Plot of log [$a(CO_2)/a(CO)$] for the reaction "$Fe_3O_4 + CO = 3\ FeO + CO_2$" as a function of reciprocal temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Ariya and others (1954)
plus	Chaudron (1921)
square	Darken and Gurry (1945)
triangle	Eastman and Evans (1924)
diamond	Fakhoury and Rosenqvist (1978)
inv tri	Garran (1928)

For part b,

circle	Kiukkola and Wagner (1957)
plus	Marion (1955)
square	Marucco and others (1970)
triangle	Matsubara (1922)
diamond	Petric and others (1981)
inv tri	Schenck and others (1927)

For part c,

circle	Schwerdtfeger and Muan (1966,1967)
plus	Touzelin (1974)
square	Trinel-Dufour and Perrot (1977)
triangle	Vallet and Raccah (1965)

Figure A.43. Plot of $\Delta_{r}H^{\circ}(298)$ for the reaction "$Fe_3O_4 + CO = 3\ FeO + CO_2$" as a function of temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Ariya and others (1954)
plus	Chaudron (1921)
square	Darken and Gurry (1945)
triangle	Eastman and Evans (1924)
diamond	Fakhoury and Rosenqvist (1978)
inv tri	Garran (1928)

For part b,

circle	Kiukkola and Wagner (1957)
plus	Marion (1955)
square	Marucco and others (1970)
triangle	Matsubara (1922)
diamond	Petric and others (1981)
inv tri	Schenck and others (1927)

For part c,

circle	Schwerdtfeger and Muan (1966,1967)
plus	Touzelin (1974)
square	Trinel-Dufour and Perrot (1977)
triangle	Vallet and Raccah (1965)

Figure A.44. Plot of log $[a(H_2O)/a(H_2)]$ for the reaction "$Fe_3O_4 + H_2 = 3\ FeO + H_2O$" as a function of reciprocal temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Bulgakova and Zaitsev (1965)
plus	Chaudron (1921)
square	Eastman and Evans (1924)
triangle	Emmett and Shultz (1930)
diamond	Marion (1955)
inv tri	Emmett and Shultz (1933)

For part b,

circle	Rau (1972)
plus	Viktorovich and others (1972)
square	Woehler and Balz (1921)
triangle	Woehler and Gunther (1923)

Figure A.45. Plot of $\Delta_{r}H^{\circ}(298)$ for the reaction "$Fe_3O_4 + H_2 = 3\ FeO + H_2O$" as a function of temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Bulgakova and Zaitsev (1965)
plus	Chaudron (1921)
square	Eastman and Evans (1924)
triangle	Emmett and Shultz (1930)
diamond	Marion (1955)
inv tri	Emmett and Shultz (1933)

For part b,

circle	Rau (1972)
plus	Viktorovich and others (1972)
square	Woehler and Balz (1921)

triangle	Woehler and Gunther (1923)

Figure A.46. Plot of E for the reaction "Fe_3O_4 + 2 Cu = 3 FeO + Cu_2O" as a function of temperature. The reaction is the net for the comparison of the wustite-magnetite and the copper-cuprite buffers. The line was calculated from the optimization. The data were taken from Kiukkola and Wagner (1957).

Figure A.47. Plot of $\Delta_r H^\circ(298)$ for the reaction "Fe_3O_4 + 2 Cu = 3 FeO + Cu_2O" as a function of temperature. The reaction is the net for the comparison of the wustite-magnetite and the copper-cuprite buffers. The line was calculated from the optimization. The data were taken from Kiukkola and Wagner (1957).

Figure A.48. Plot of E for the reaction "Fe_3O_4 + Ni = 3 FeO + NiO" as a function of temperature. The reaction is the net for the comparison of the wustite-magnetite and the nickel-bunsenite buffers. The line was calculated from the optimization. The sources of data are as follows:

circle	Asao and others (1970)
plus	Bonnet and Perrin (1978)
square	Charette (1967)
triangle	Roeder and Smeltzer (1964)
diamond	Saito and others (1972)

Figure A.49. Plot of $\Delta_r H^\circ(298)$ for the reaction "Fe_3O_4 + Ni = 3 FeO + NiO" as a function of temperature. The reaction is the net for the comparison of the wustite-magnetite and the nickel-bunsenite buffers. The line was calculated from the optimization. The sources of data are as follows:

circle	Asao and others (1970)
plus	Bonnet and Perrin (1978)
square	Charette (1967)
triangle	Roeder and Smeltzer (1964)
diamond	Saito and others (1972)

Figure A.50. Plot of log K for the reaction "2 Fe_3O_4 + 0.5 O_2 = 3 Fe_2O_3" as a function of reciprocal temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Chizhikov and others (1971)
plus	Darken and Gurry (1946)
square	Komarov and others (1967)
triangle	Kurepin (1975)
diamond	Myers and Eugster (1983)
inv tri	Norton (1955)

For part b,

circle	Schmahl and others (1969)
plus	Schmahl (1951)
square	Schwab and ~~Kuenster~~ (1981) Kuestner
triangle	Smiltens (1957)

diamond	Snethlage and Schrocke (1976)
inv tri	Treadwell (1916)

For part c,

circle	Tretyakov and Khomyakov (1962)
plus	Tretyakov and others (1977)
square	White and Richards (1949)

Figure A.51. Plot of $\Delta_{r}H^{\circ}(298)$ for the reaction "2 Fe_3O_4 + 0.5 O_2 = 3 Fe_2O_3" as a function of temperature. The line was calculated from the optimization. The sources of data are as follows: For part a,

circle	Chizhikov and others (1971)
plus	Darken and Gurry (1946)
square	Komarov and others (1967)
triangle	Kurepin (1975)
diamond	Myers and Eugster (1983)
inv tri	Norton (1955)

For part b,

circle	Schmahl and others (1969)
plus	Schmahl (1951)
square	Schwab and ~~Kuenster~~ (1981) Kuestner
triangle	Smiltens (1957)
diamond	Snethlage and Schrocke (1976)
inv tri	Treadwell (1916)

For part c,

circle	Tretyakov and Khomyakov (1962)
plus	Tretyakov and others (1977)
square	White and Richards (1949)

Figure A.52. Plot of log K for the reaction "3 Fe_2O_3 + H_2 = 2 Fe_3O_4 + H_2O" as a function of reciprocal temperature. The line was calculated from the optimization. The sources of data are as follows:

circle	Rau (1972)
plus	Woehler and Balz (1921)
square	Woehler and Gunther (1932)

The sigmoid shape of the curve appears to be anomalous. However, it is a result of the lambda anomalies in magnetite and hematite at 849 and 955 K, respectively.

Figure A.53. Plot of $\Delta_{r}H^{\circ}(298)$ for the reaction "3 Fe_2O_3 + H_2 = 2 Fe_3O_4 + H_2O" as a function of temperature. The line was calculated from the optimization. The sources of data are as follows:

circle	Rau (1972)
plus	Woehler and Balz (1921)
square	Woehler and Gunther (1932)

Figure A.54. Plot of E for the reaction "3 Fe_2O_3 + 2 Cu = 2 Fe_3O_4 + Cu_2O" as a function of temperature. The reaction is the net for the comparison of the hematite-magnetite and the copper-cuprite buffers. The line was calculated from the optimization. The sources of data are as follows:

circle	Bonnet and Perrin (1978)
plus	Bryant and Smeltzer (1969)
square	Fitzner (1979)
triangle	Ramana Rao and Tare (1972)
diamond	Ramana Rao and Tare (1973)

Figure A.55. Plot of $\Delta_r H^\circ(298)$ for the reaction "3 Fe_2O_3 + 2 Cu = 2 Fe_3O_4 + Cu_2O" as a function of temperature. The reaction is the net for the comparison of the hematite-magnetite and the copper-cuprite buffers. The line was calculated from the optimization. The sources of data are as follows:

circle	Bonnet and Perrin (1978)
plus	Bryant and Smeltzer (1969)
square	Fitzner (1979)
triangle	Ramana Rao and Tare (1972)
diamond	Ramana Rao and Tare (1973)

Figure A.56. Plot of E for the reaction "3 Fe_2O_3 + Ni = 2 Fe_3O_4 + NiO" as a function of temperature. The reaction is the net for the comparison of the hematite-magnetite and the nickel-bunsenite buffers. The line was calculated from the optimization. The sources of data are as follows:

circle	Charette (1967)
plus	Moriyama and others (1969)
square	Saito and others (1972)

The measurements by Trumm (1981) and Ulmer and others (1976) were at elevated pressure and were not plotted on this figure.

Figure A.57. Plot of $\Delta_r H^\circ(298)$ for the reaction "3 Fe_2O_3 + Ni = 2 Fe_3O_4 + NiO" as a function of temperature. The reaction is the net for the comparison of the hematite-magnetite and the nickel-bunsenite buffers. The line was calculated from the optimization. The sources of data are as follows:

circle	Charette (1967)
plus	Moriyama and others (1969)
square	Saito and others (1972)
triangle	Trumm (1981)
diamond	Ulmer and others (1976)

Figure A.58. Plot of E for the reaction "3 Fe_2O_3 + Fe = 2 Fe_3O_4 + FeO" as a function of temperature. The reaction is the net for the comparison of the hematite-magnetite and the iron-wustite buffers. The line was calculated from the optimization. The sources of data are as follows:

circle	Blumenthal (1961)
plus	Gordeev and Tretyakov (1963)
square	Jacobsson (1985)

Figure A.59. Plot of $\Delta_r H°(298)$ for the reaction "3 Fe_2O_3 + Fe = 2 Fe_3O_4 + FeO" as a function of temperature. The reaction is the net for the comparison of the hematite-magnetite and the iron-wustite buffers. The line was calculated from the optimization. The sources of data are as follows:

circle	Blumenthal (1961)
plus	Gordeev and Tretyakov (1963)
square	Jacobsson (1985)

Figure A.60. Pressure-temperature plot showing the stability fields of the three polymorphs of Fe_2SiO_4. The lines were calculated from the results of the optimization. The invariant point is near 1823 K (1550°C) and 66 kbars. The sources of data are as follows:

circle	Akimoto and others (1967)
plus	Akimoto and others (1977)
square	Akimoto and Yagi (1986)
triangle	Hsu (1967)
diamond	Lindsley (1967)
inv tri	Ohtani and others (1979)

Figure A.61. Plot of log K for the reaction "Fe_2SiO_4 = 2 Fe + SiO_2 + O_2" as a function of reciprocal temperature. The line was calculated from the optimization. The sources of data are as follows:

circle	Kitayama and Katsura (1968)
plus	Myers and Eugster (1983)
square	Nafziger and Muan (1967)
triangle	Schwab and ~~Kuenster~~ (1981) Kuestner
diamond	Taylor and Schmalzried (1964)
"x"	Williams (1971)

Figure A.62. Plot of $\Delta_r H°(298)$ for the reaction "Fe_2SiO_4 = 2 Fe + SiO_2 + O_2" as a function of temperature. The line was calculated from the optimization. The sources of data are as follows:

circle	Kitayama and Katsura (1968)
plus	Myers and Eugster (1983)
square	Nafziger and Muan (1967)
triangle	Schwab and ~~Kuenster~~ (1981) Kuestner
diamond	Taylor and Schmalzried (1964)
"x"	Williams (1971)

Figure A.63. Plot of log K for the reaction "$0.5\ Fe_2SiO_4 + CO = Fe + 0.5\ SiO_2 + CO_2$" as a function of reciprocal temperature. The line was calculated from the optimization. The sources of data are as follows:

circle	Lebedev and Levitsky (1962)
plus	Schenck and others (1932)
square	Schwerdtfeger and Muan (1966)

Figure A.64. Plot of $\Delta_r H^\circ(298)$ for the reaction "$0.5\ Fe_2SiO_4 + CO = Fe + 0.5\ SiO_2 + CO_2$" as a function of temperature. The line was calculated from the optimization. The sources of data are as follows:

circle	Lebedev and Levitsky (1962)
plus	Schenck and others (1932)
square	Schwerdtfeger and Muan (1966)

Figure A.65. Plot of log K for the reaction "$0.5\ Fe_2SiO_4 + H_2 = Fe + 0.5\ SiO_2 + H_2O$" as a function of reciprocal temperature. The line was calculated from the optimization. The data were taken from the study by Berliner and Shapovlova (1966).

Figure A.66. Plot of $\Delta_r H^\circ(298)$ for the reaction "$0.5\ Fe_2SiO_4 + H_2 = Fe + 0.5\ SiO_2 + H_2O$" as a function of temperature. The line was calculated from the optimization. The data were taken from the study by Berliner and Shapovlova (1966).

Figure A.67. Plot of E for the reaction "$FeO + 0.5\ SiO_2 = 0.5\ Fe_2SiO_4$" as a function of temperature. The reaction is the net for the comparison of the iron-wustite and the quartz-fayalite-iron buffers. The line was calculated from the optimization. The sources of data are as follows:

circle	Levitski and Ratiani (1970)
plus	Shiomi and others (1975)
square	O'Neill (1987)

Figure A.68. Plot of $\Delta_r H^\circ(298)$ for the reaction "$FeO + 0.5\ SiO_2 = 0.5\ Fe_2SiO_4$" as a function of temperature. The reaction is the net for the comparison of the iron-wustite and the quartz-fayalite-iron buffers. The line was calculated from the optimization. The sources of data are as follows:

circle	Levitski and Ratiani (1970)
plus	Shiomi and others (1975)
square	O'Neill (1987)

Figure A.69. Plot of E for the reaction "$2\ Fe + SiO_2 + 2\ Fe_3O_4 = Fe_2SiO_4 + 6\ FeO$" as a function of temperature. The line was calculated from the optimization. The data were taken from the study by Eremenko and Filippov (1967). The equation supplied by these authors must be erroneous.

Figure A.70. Plot of log K for the reaction "$Fe_3O_4 + 1.5\ SiO_2 = 1.5\ Fe_2SiO_4 + 0.5\ O_2$" as a function of reciprocal temperature. The line was calculated from the optimization. The sources of data are as follows:

circle	Myers and Eugster (1983)
plus	Schwab and ~~Kuenster~~ (1981) Kuestner
square	Schwab and Sohnlein (1977)

Figure A.71. Plot of $\Delta_r H^\circ(298)$ for the reaction "$Fe_3O_4 + 1.5\ SiO_2 = 1.5\ Fe_2SiO_4 + 0.5\ O_2$" as a function of temperature. The line was calculated from the optimization. The sources of data are as follows:

circle	Myers and Eugster (1983)
plus	Schwab and ~~Kuenster~~ (1981) Kuestner
square	Schwab and Sohnlein (1977)

From the plot, it may be concluded that parts of the experimental data by Schwab and coworkers were not equilibrium observations.

Figure A.72. Plot of log K for the reaction "$Fe_3O_4 + 1.5\ SiO_2 + CO = 1.5\ Fe_2SiO_4 + CO_2$" as a function of reciprocal temperature. The line was calculated from the results of the optimization. The sources of data are as follows:

circle	Schenck and others (1932)
plus	Schwerdtfeger and Muan (1966)

Figure A.73. Plot of $\Delta_r H^\circ(298)$ for the reaction "$Fe_3O_4 + 1.5\ SiO_2 + CO = 1.5\ Fe_2SiO_4 + CO_2$" as a function of temperature. The line was calculated from the results of the optimization. The sources of data are as follows:

circle	Schenck and others (1932)
plus	Schwerdtfeger and Muan (1966)

Figure A.74. Plot of $\Delta_r H^\circ(298)$ for the reaction "$Fe_3O_4 + 1.5\ SiO_2 + H_2 = 1.5\ Fe_2SiO_4 + H_2O$" as a function of temperature. The line was calculated from the optimization. The sources of data are as follows:

circle	Hewitt (1978)
plus	Myers and Eugster (1983)
square	Wones and Gilbert (1969)

Figure A.75. Plot of E for the reaction "Fe_3O_4 + 1.5 SiO_2 + 2 Cu = 1.5 Fe_2SiO_4 + Cu_2O" as a function of temperature. The reaction is the net for the comparison of the quartz-fayalite-magnetite and the copper-cuprite buffers. The line was calculated from the results of the optimization. The data were taken from the study by O'Neill (1987).

Figure A.76. Plot of $\Delta_r H°(298)$ for the reaction "Fe_3O_4 + 1.5 SiO_2 + 2 Cu = 1.5 Fe_2SiO_4 + Cu_2O" as a function of temperature. The reaction is the net for the comparison of the quartz-fayalite-magnetite and the copper-cuprite buffers. The line was calculated from the results of the optimization. The data were taken from the study by O'Neill (1987).

Figure A.77. Plot of E for the reaction "Fe_3O_4 + 1.5 SiO_2 + Fe = 1.5 Fe_2SiO_4 + FeO" as a function of temperature. The reaction is the net for the comparison of the quartz-fayalite-magnetite and the iron-wustite buffers. The line was calculated from the optimization. The data were taken from the study by Schwab and Sohnlein (1977).

Figure A.78. Plot of $\Delta_r H°(298)$ for the reaction "Fe_3O_4 + 1.5 SiO_2 + Fe = 1.5 Fe_2SiO_4 + FeO" as a function of temperature. The reaction is the net for the comparison of the quartz-fayalite-magnetite and the iron-wustite buffers. The line was calculated from the optimization. The data were taken from the study by Schwab and Sohnlein (1977).

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Recommended Standard Electrochemical Potentials and Fugacities of Oxygen for the Solid Buffers and Thermodynamic Data in the Systems Iron-Silicon-Oxygen, Nickel-Oxygen, and Copper-Oxygen

Part 4. Figures

John L. Haas, Jr.
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National Center, Mail Stop 959
Reston, Virginia 22092
U.S.A.

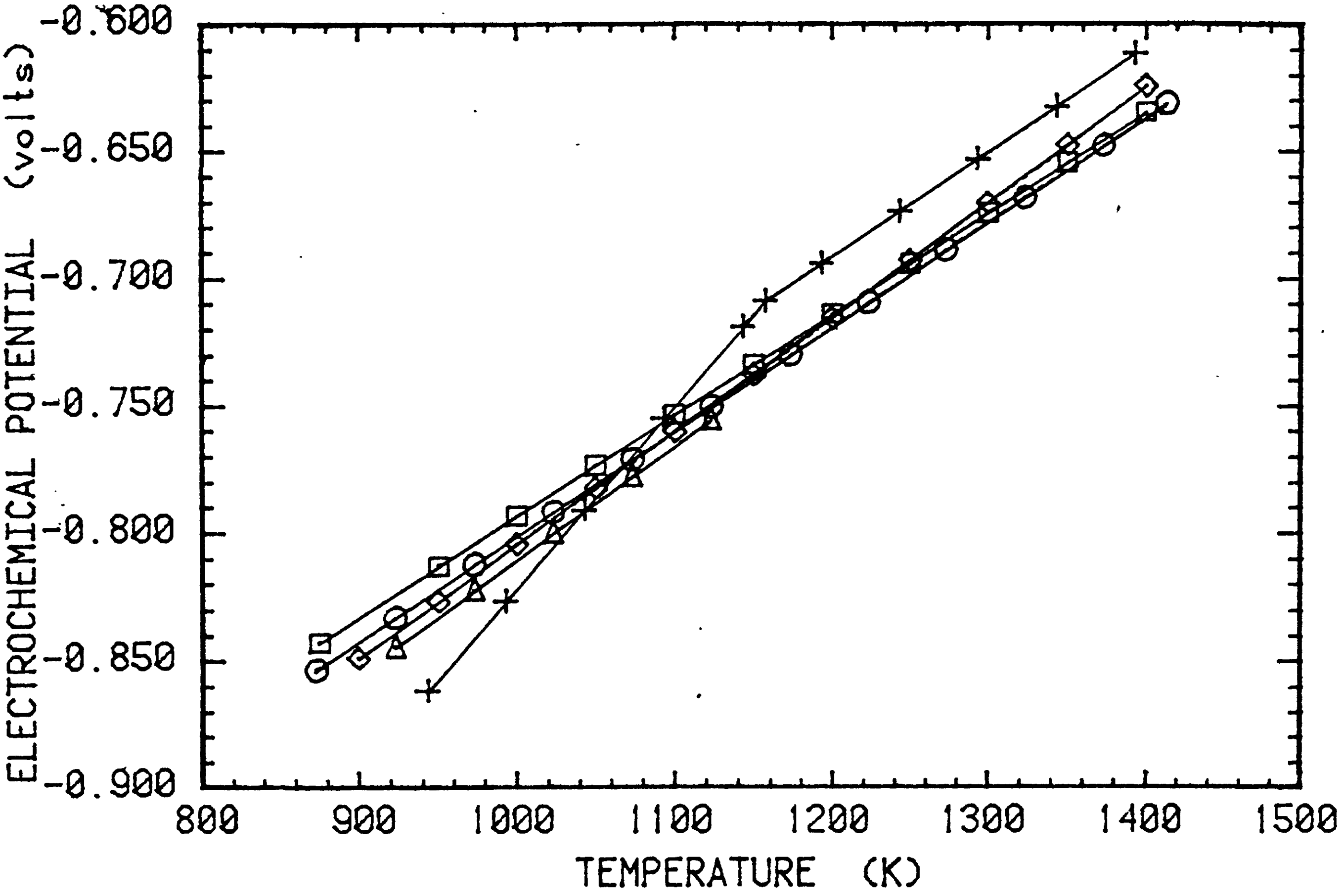
January 17, 1988

Recommended fugacities and standard electrochemical potentials for O_2 in the buffer pairs from 200 to 1800 K were derived from critical reviews of experimental data and thermodynamic theory. Included are C_p°, H°(T)-H°(298), [G°(T) -H°(298)]/T, S°, $\Delta_f H^\circ$, $\Delta_f G^\circ$, V°, and the coefficients of volume expansion and of volume compression for the oxide phases.

Planned for publication as a Bulletin of the U.S. Geological Survey. This report is not to be used nor cited without prior permission by the author (Phone 703+648-6755). Scientific review of this version (text and tables Jan. 17, 1988; figures Dec. 1, 1987) has not been completed and, therefore, the manuscript is subject to change.

J.L. Haas, Jr., "Oxygen Buffers" 1-Dec-87

Figure 1.1



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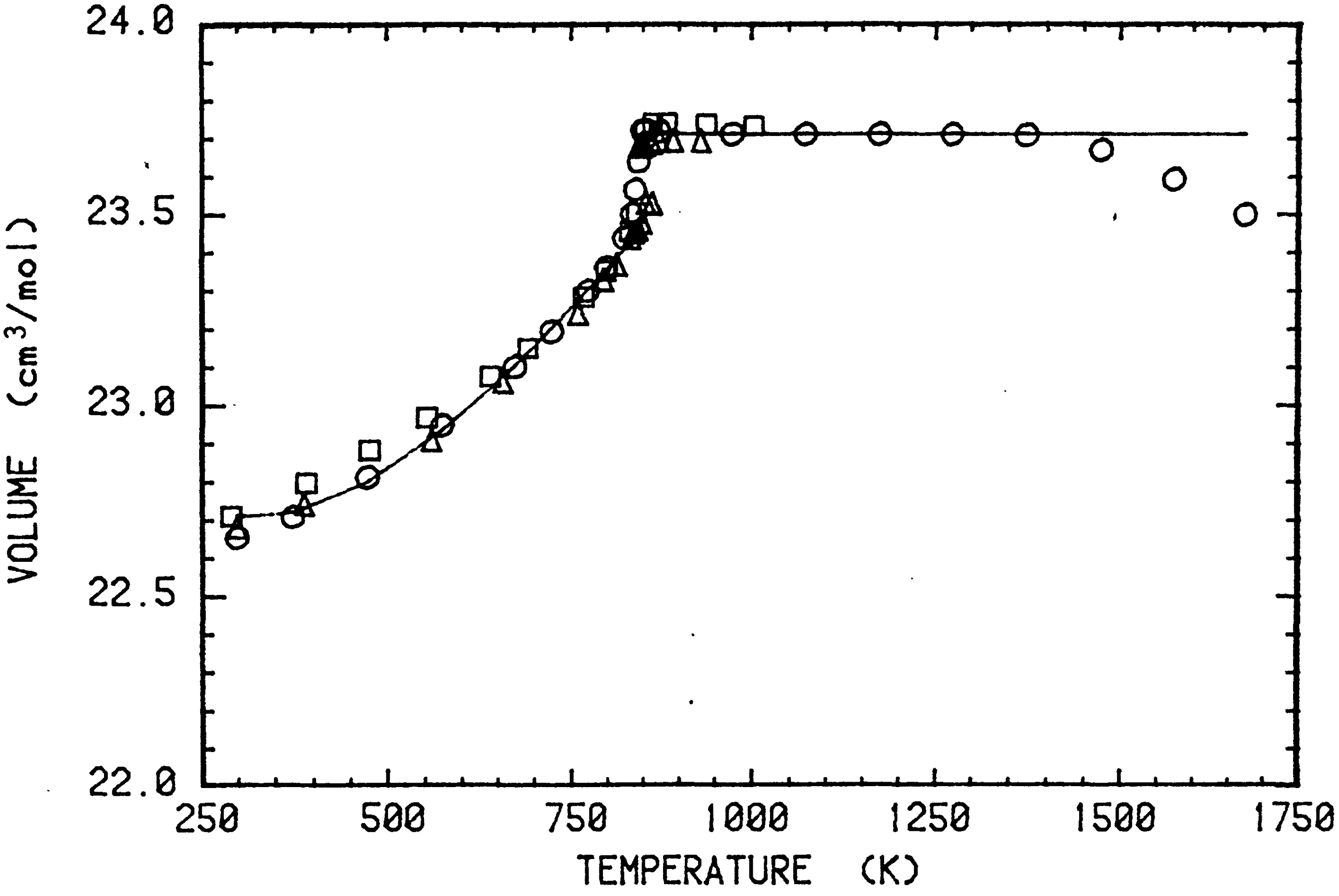
J.L. Haas, Jr., "Oxygen Buffers" 1-Dec-87

Figure 3.1



J.L. Haas, Jr., "Oxygen Buffers" 1-Dec-87

Figure 3.2

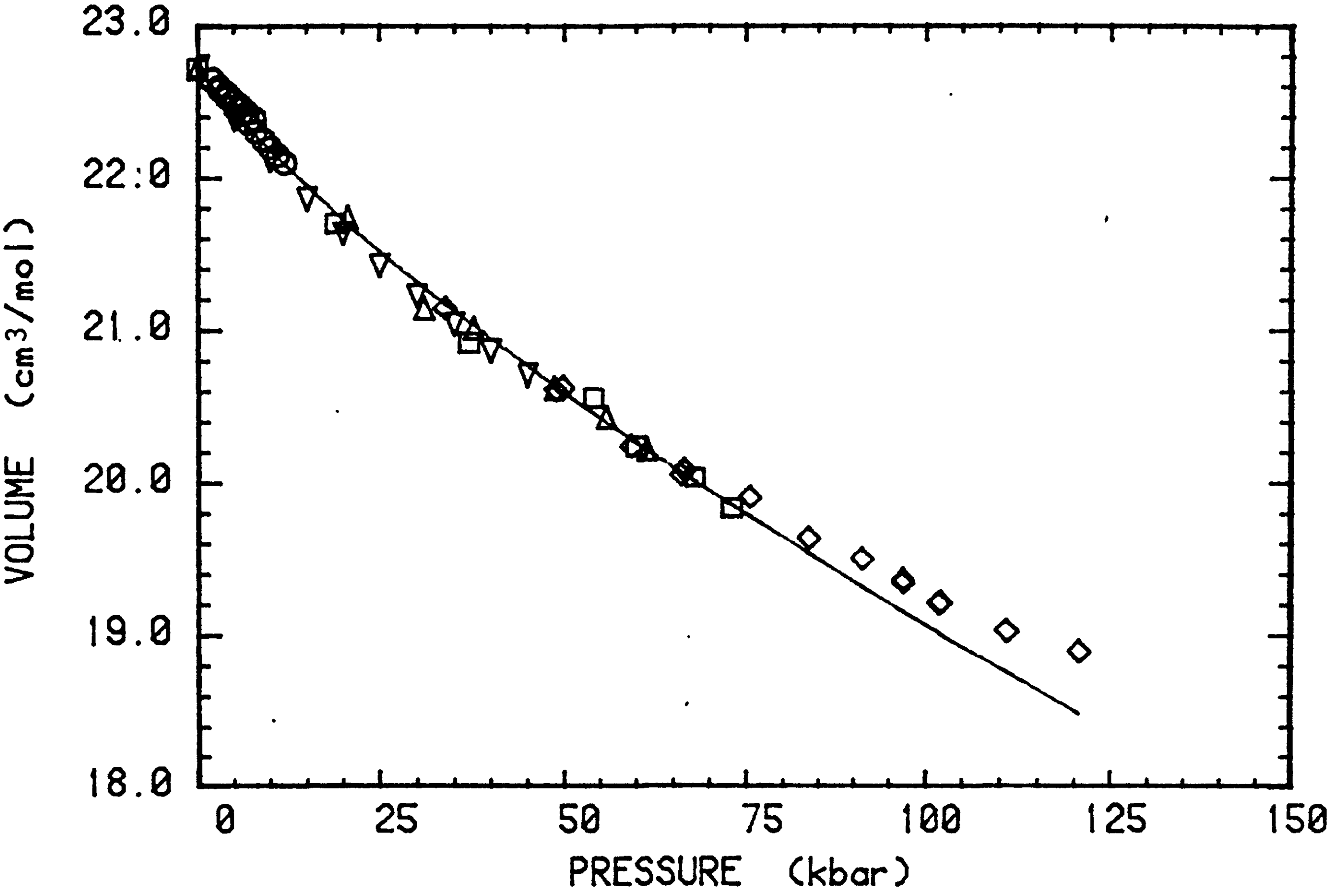


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Figure 3.3

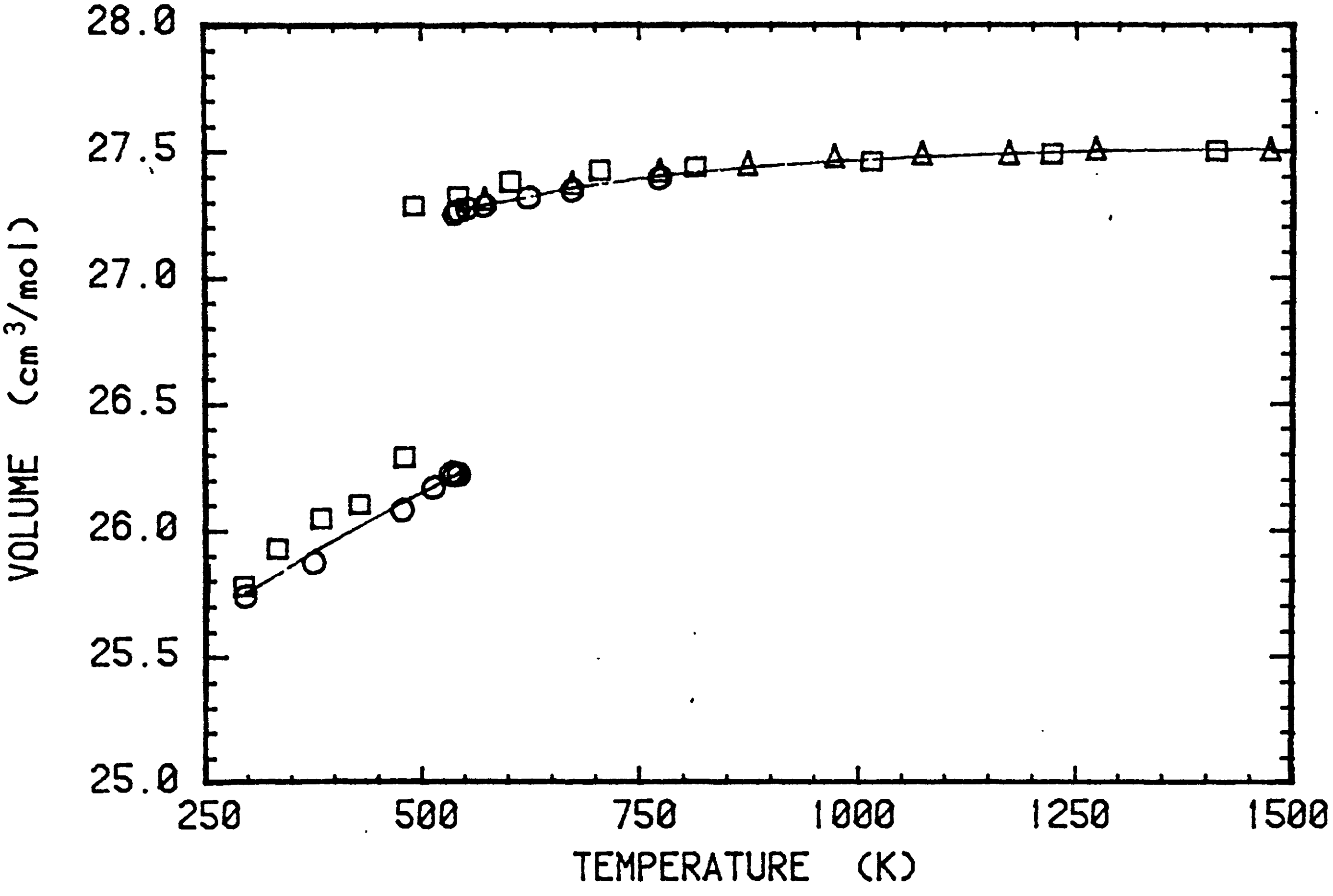

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Figure 3.4

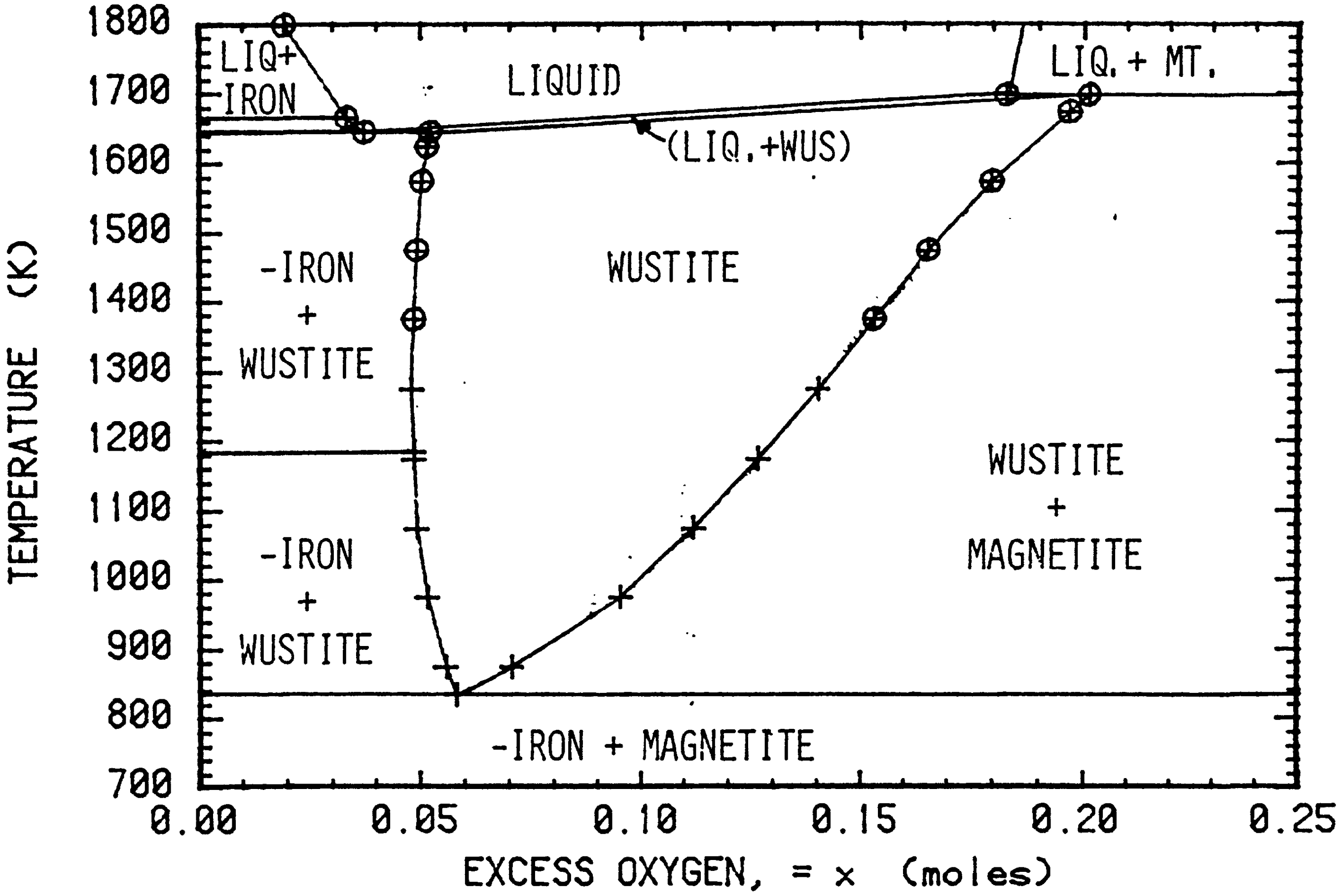

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Figure 5.1

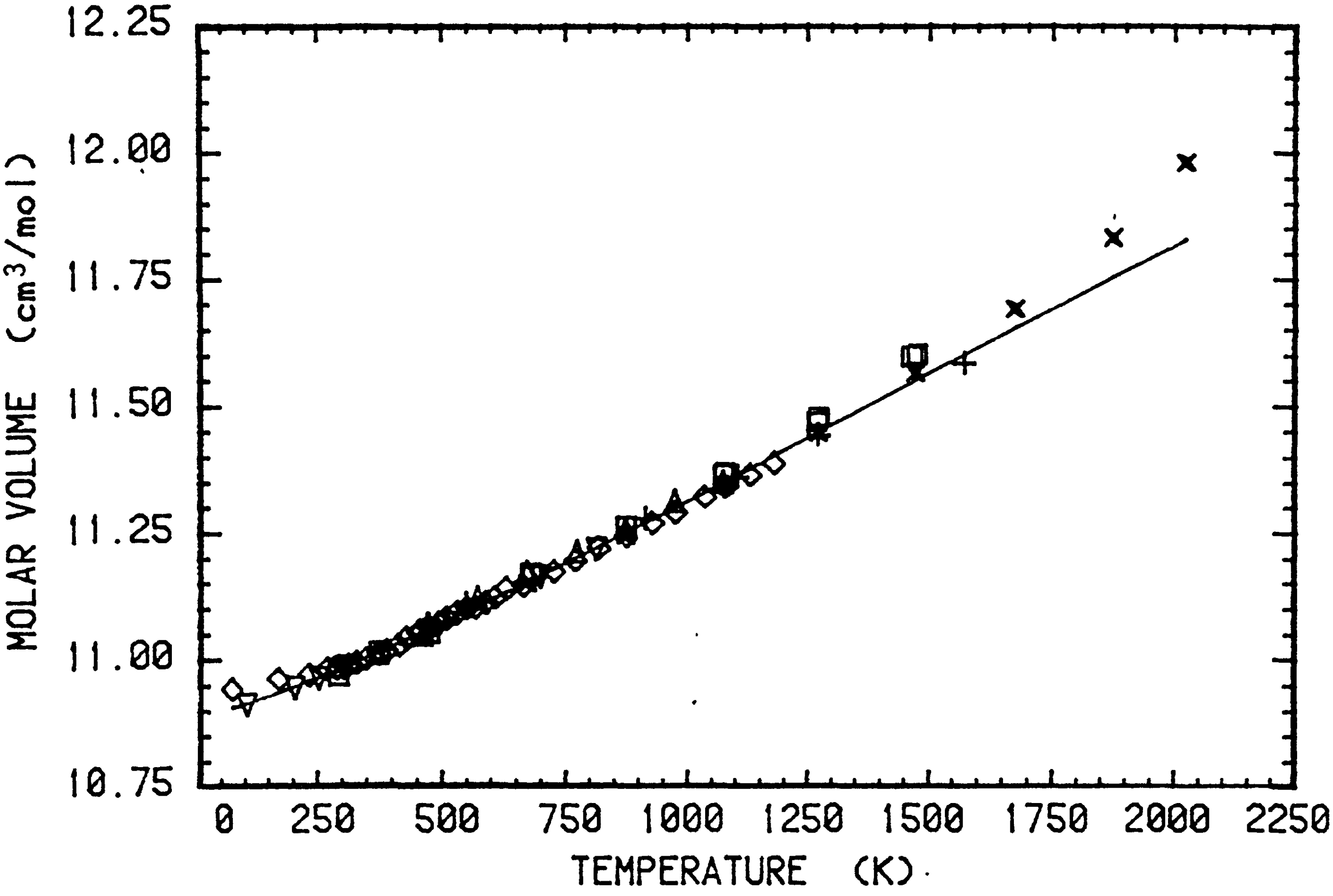
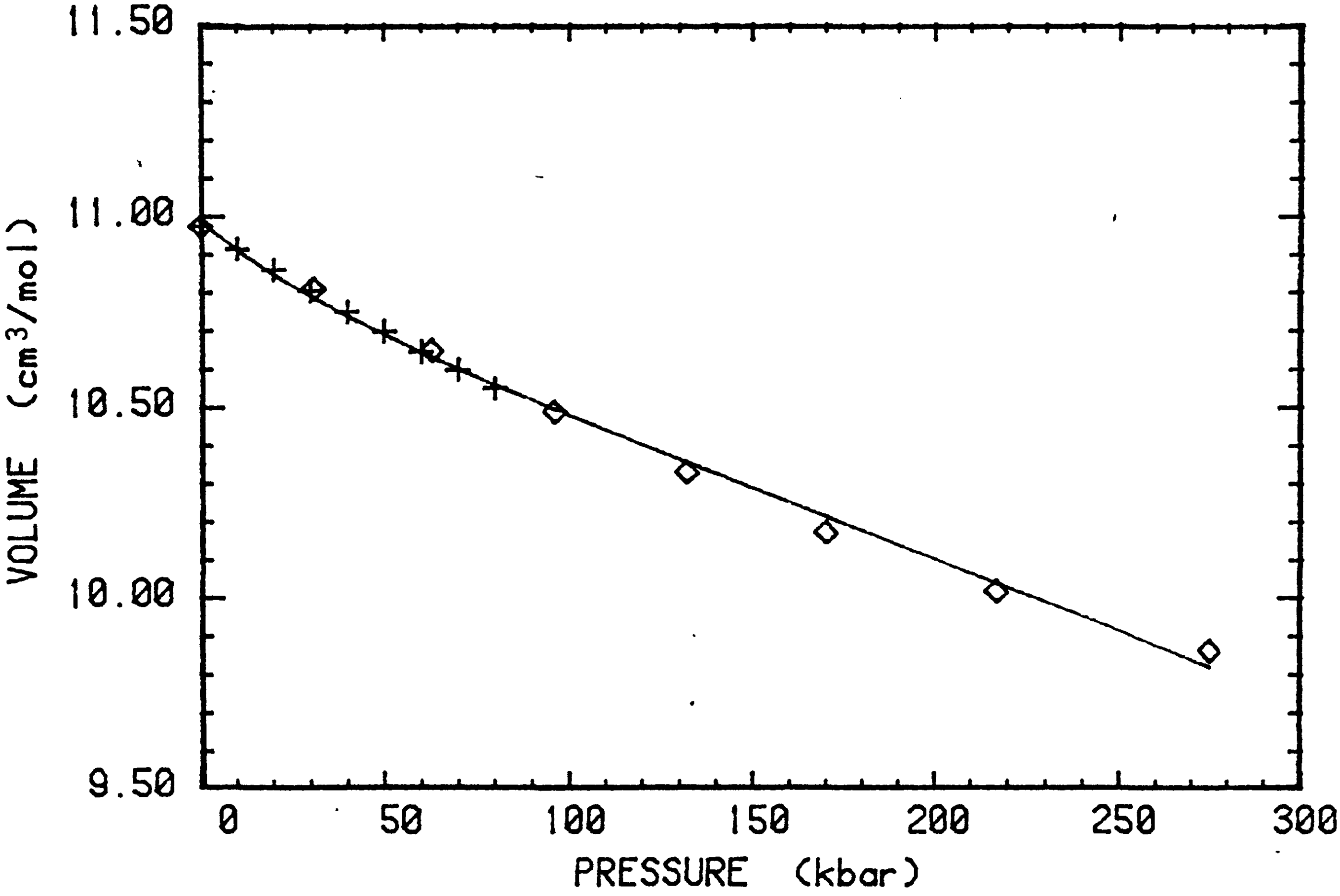
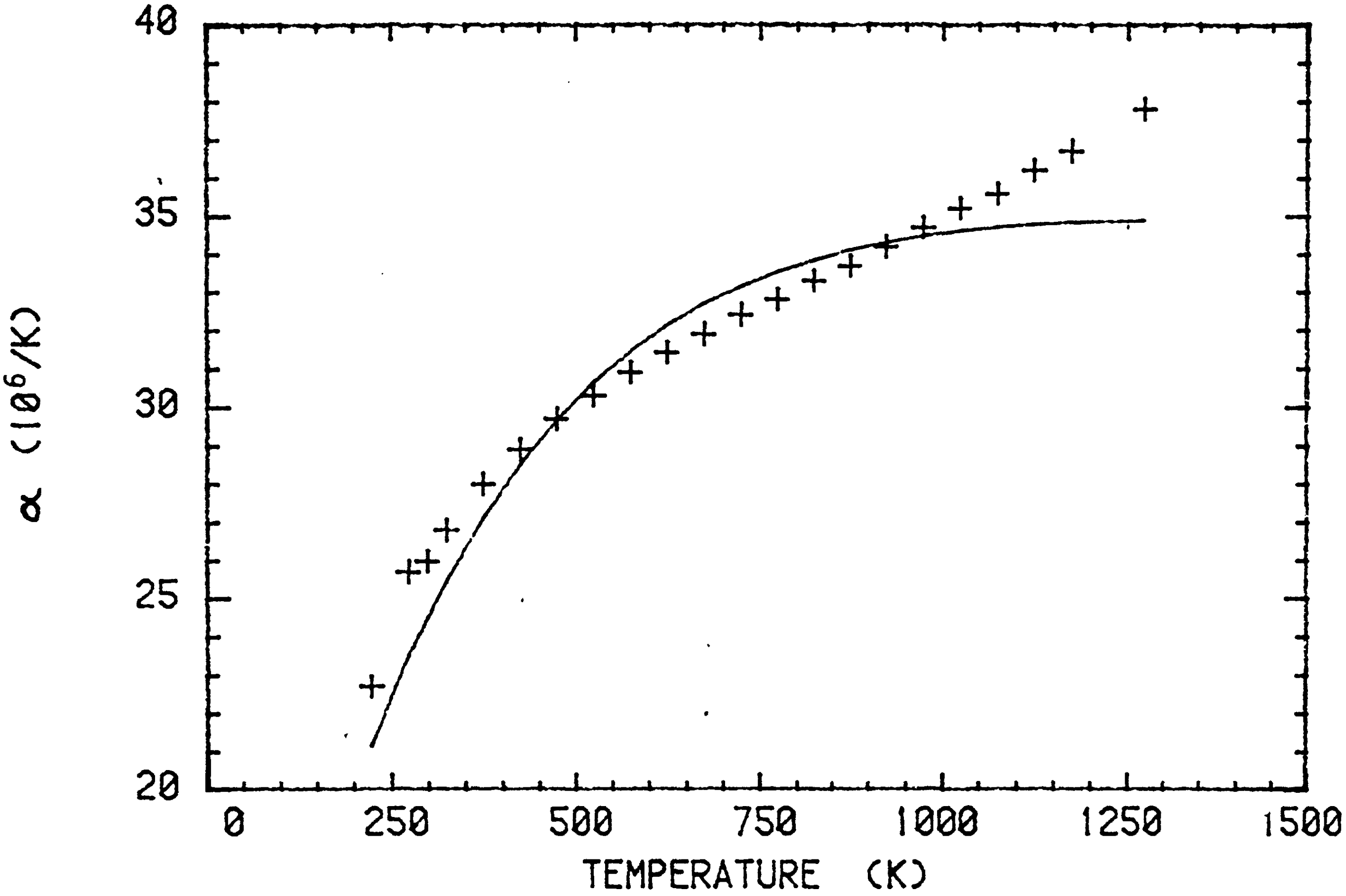


Figure 5.2


11.50
11.00
10.50
10.00
9.50
VOLUME (cm^3/mol)
0
50
100
150
200
250
300
PRESSURE (kbar)

J.L. Haas, Jr., 'oxygen Buffers' 1-Dec-87

Figure 5.3



J.L. Haas, Jr., 'Oxygen Buffers' 1-Dec-87

Figure 5.4

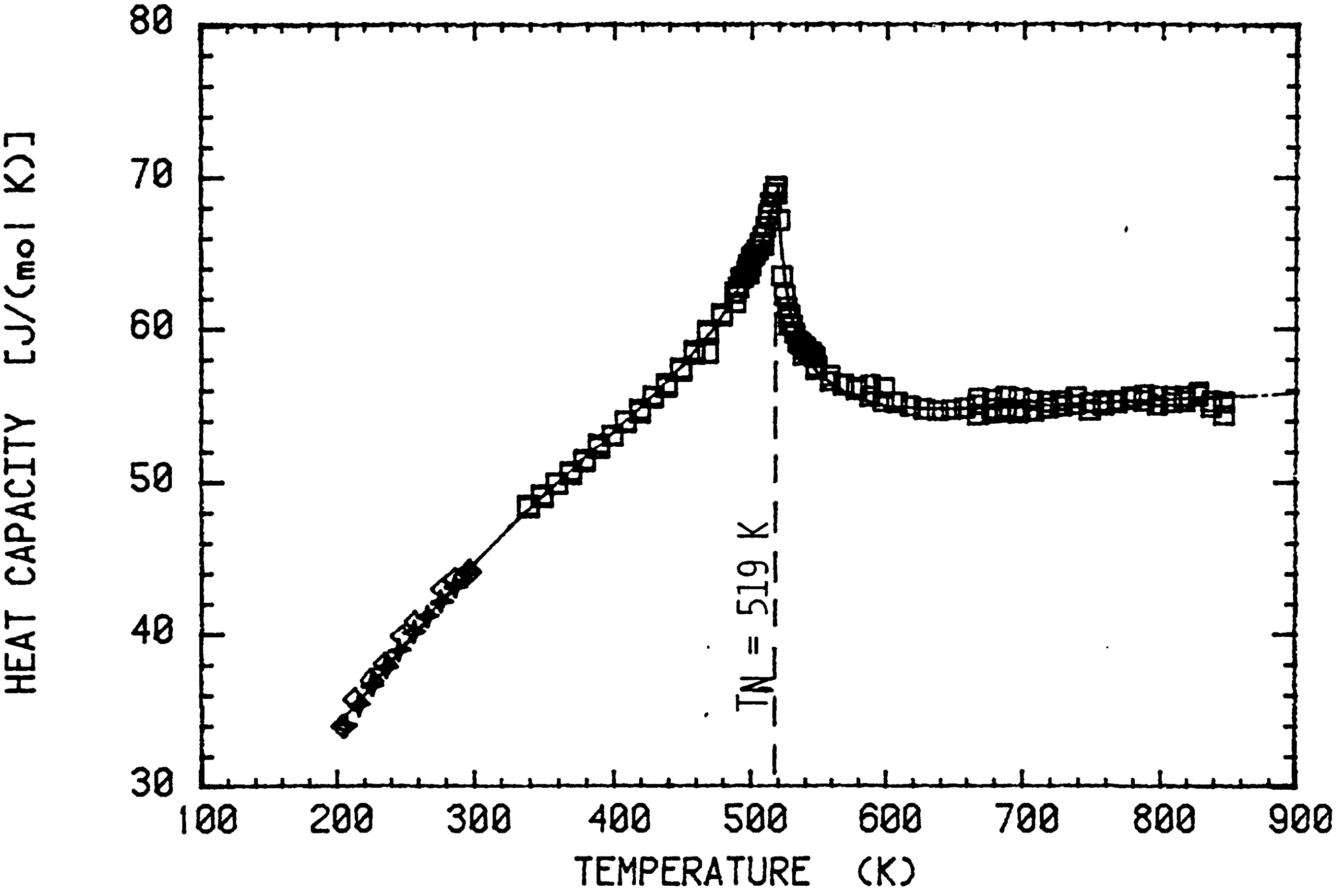


Figure 5.5

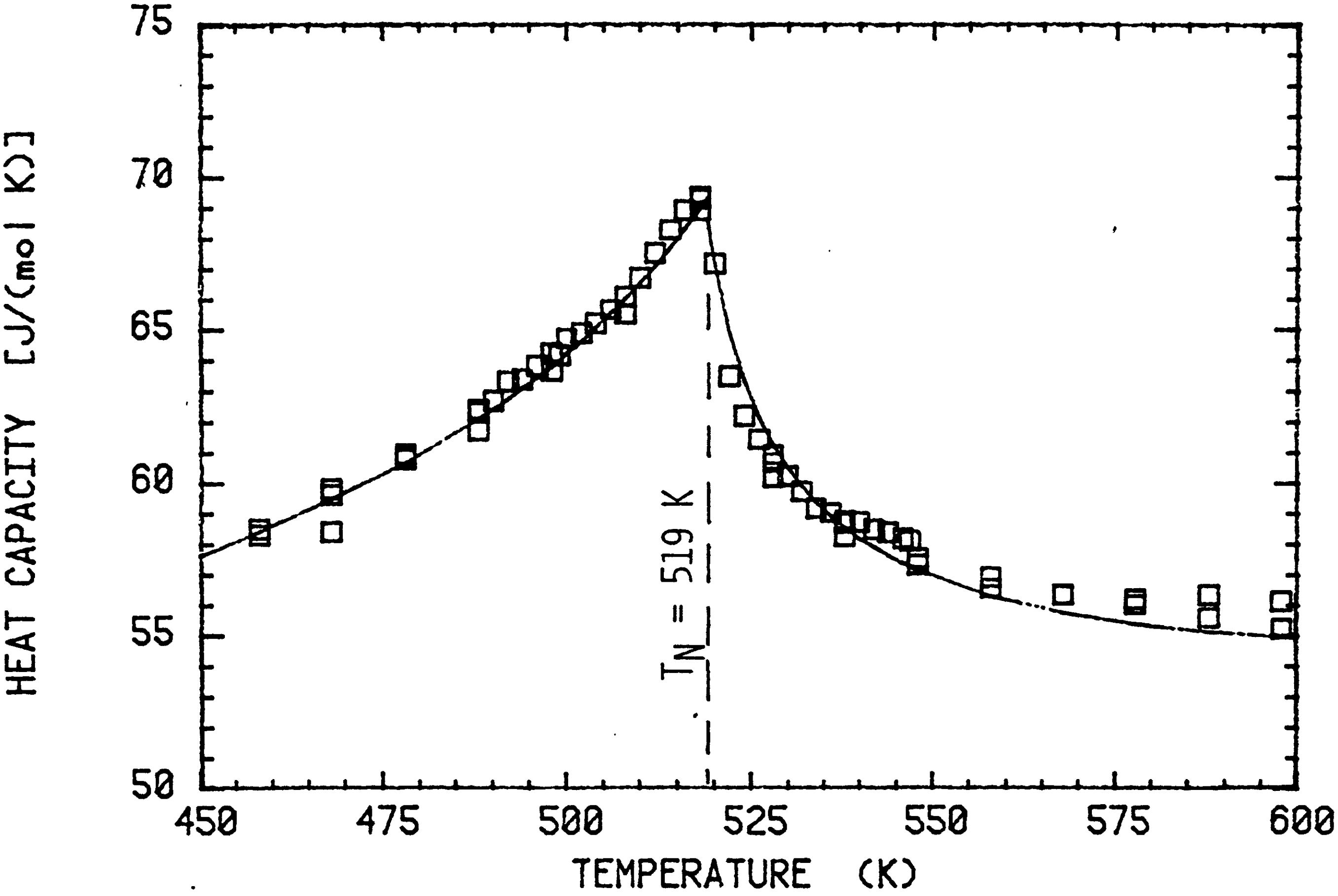
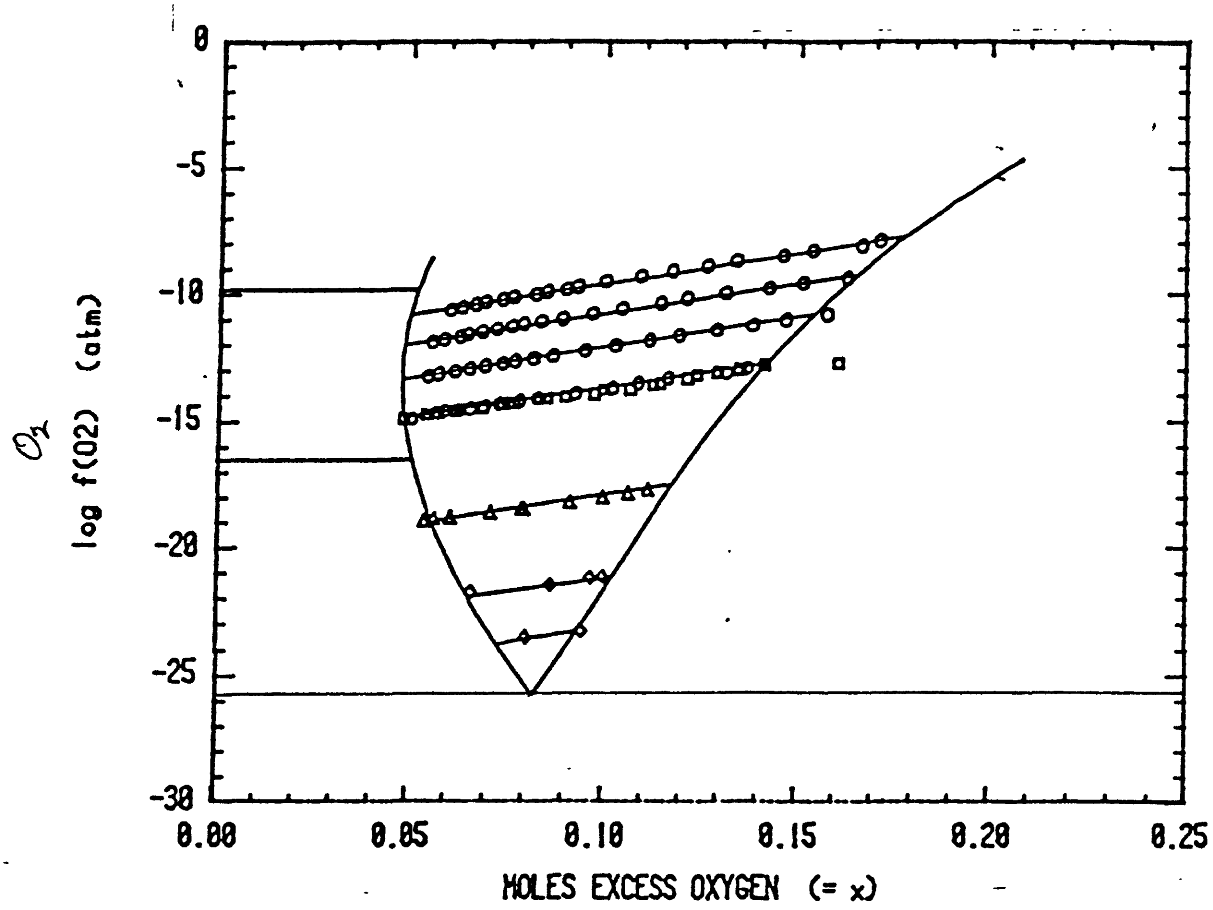

75
70
65
60
55
50
450
475
500
525
550
575
600
HEAT CAPACITY [J/(mol K)]
TEMPERATURE (K)
T_N = 519 K

Figure 5.6


0
-5
-10
-15
-20
-25
-30
O_2
log f(O2) (atm)
0.00
0.05
0.10
0.15
0.20
0.25
MOLES EXCESS OXYGEN (= x)

J.L. Haas, Jr., "Oxygen Buffers" 1-Dec-87

Figure 7.01

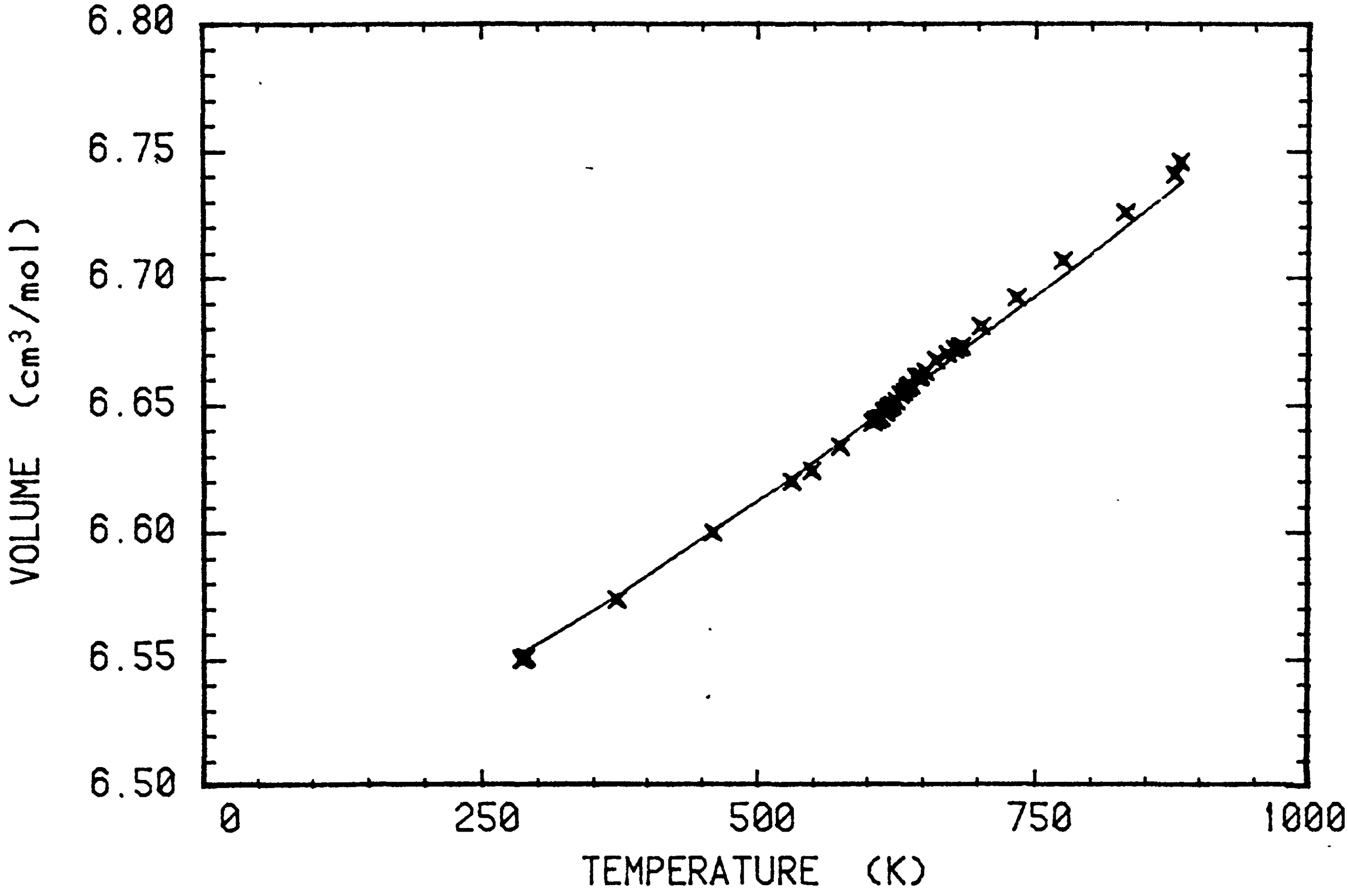


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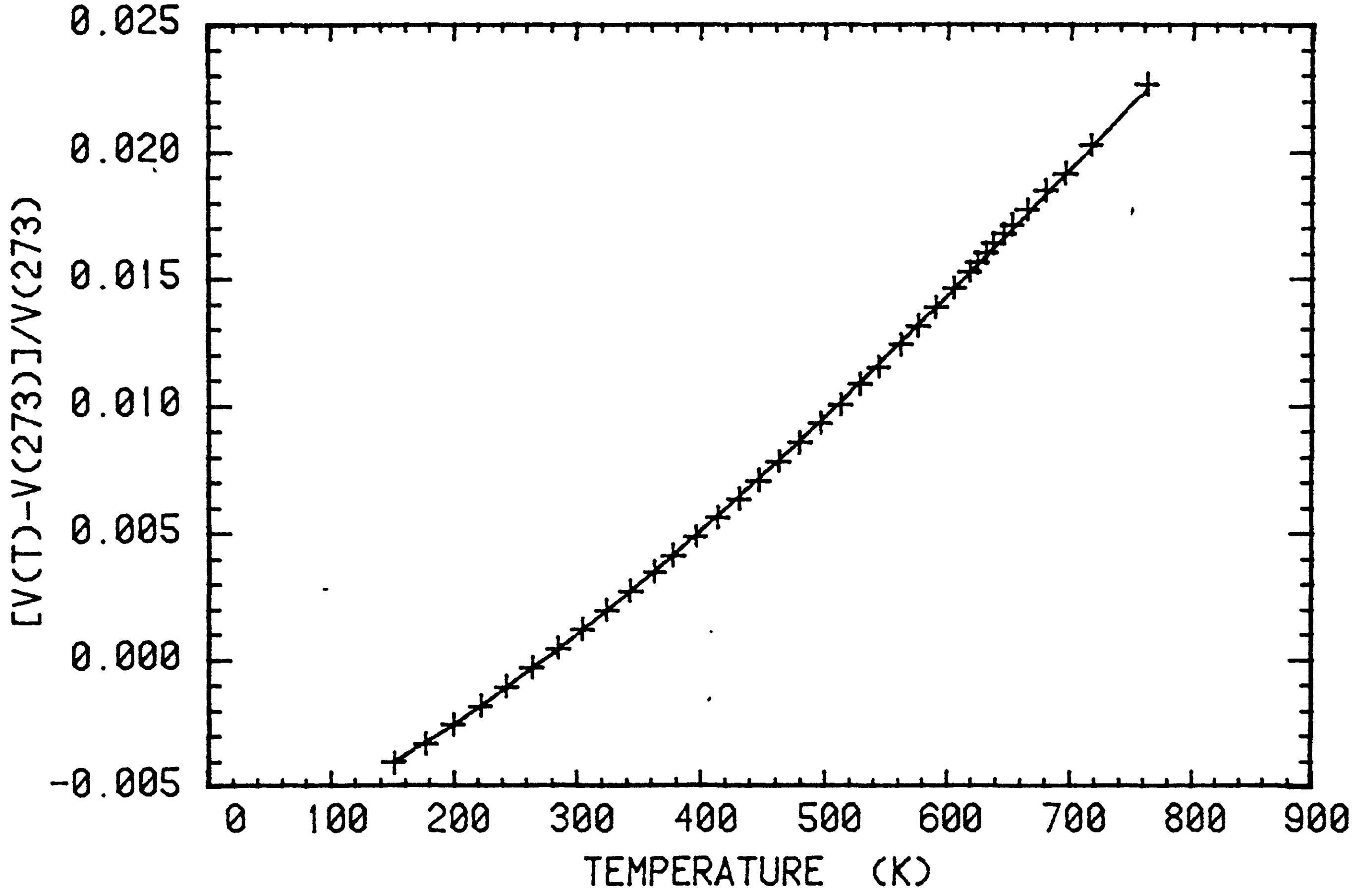
Figure 7.02



J.L. Haas, Jr., 'Oxygen Buffers' 1-Dec-87

Figure 7.03

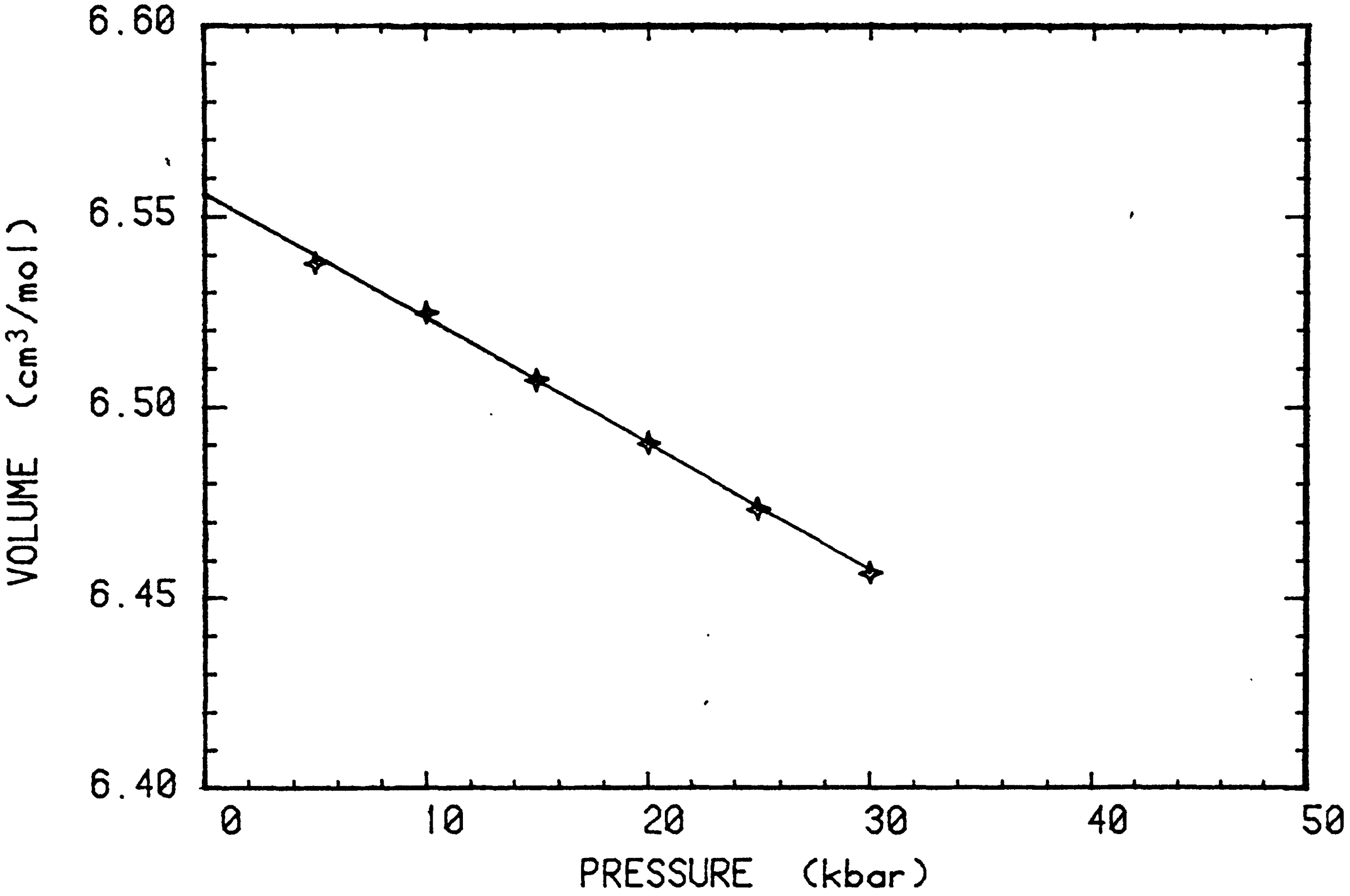


Figure 7.04

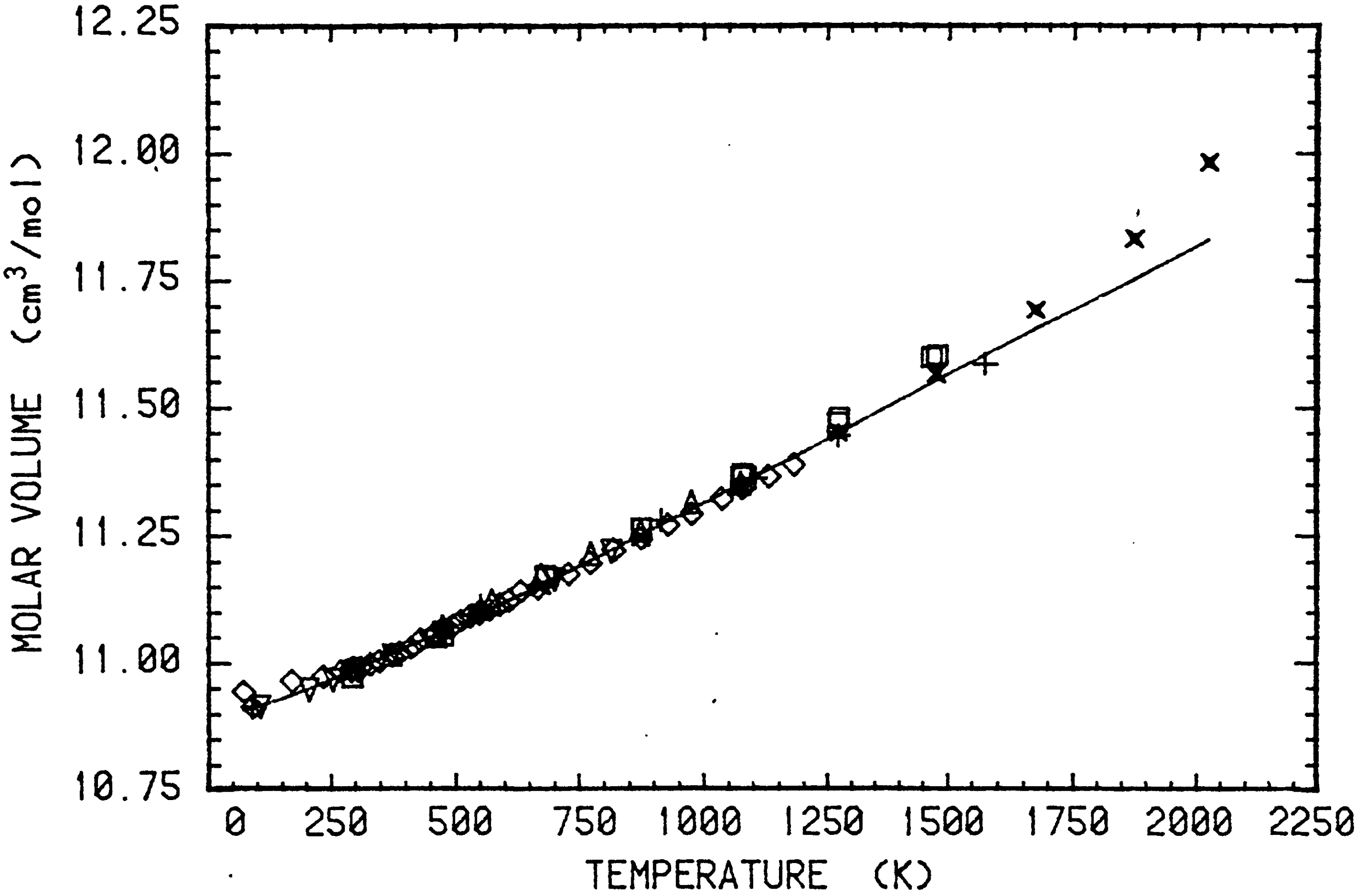

12.25
12.00
11.75
11.50
11.25
11.00
10.75
MOLAR VOLUME (cm^3/mol)
0
250
500
750
1000
1250
1500
1750
2000
2250
TEMPERATURE (K)

Figure 7.05

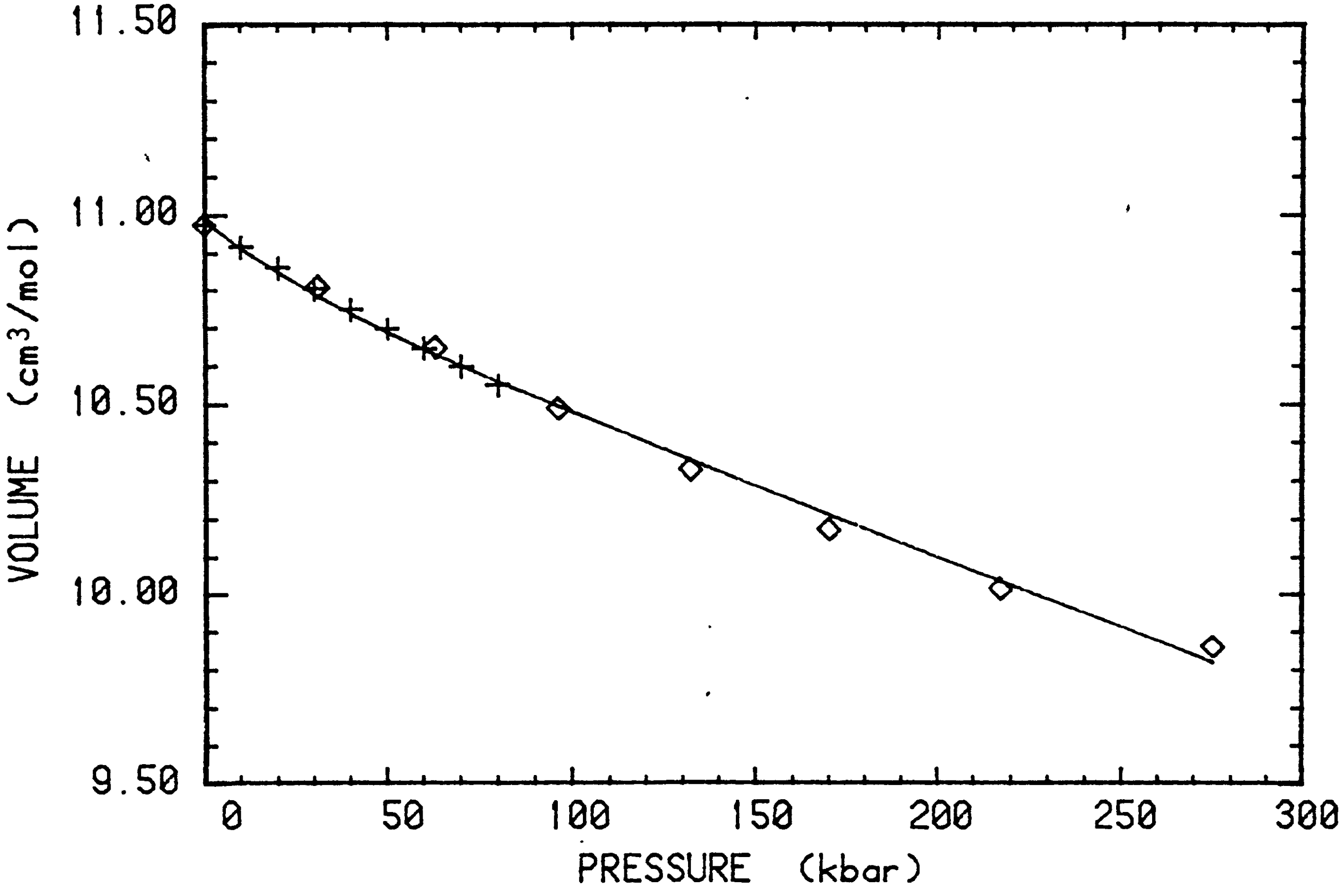

11.50
11.00
10.50
10.00
9.50
VOLUME (cm^3/mol)
0
50
100
150
200
250
300
PRESSURE (kbar)

Figure 7.06,

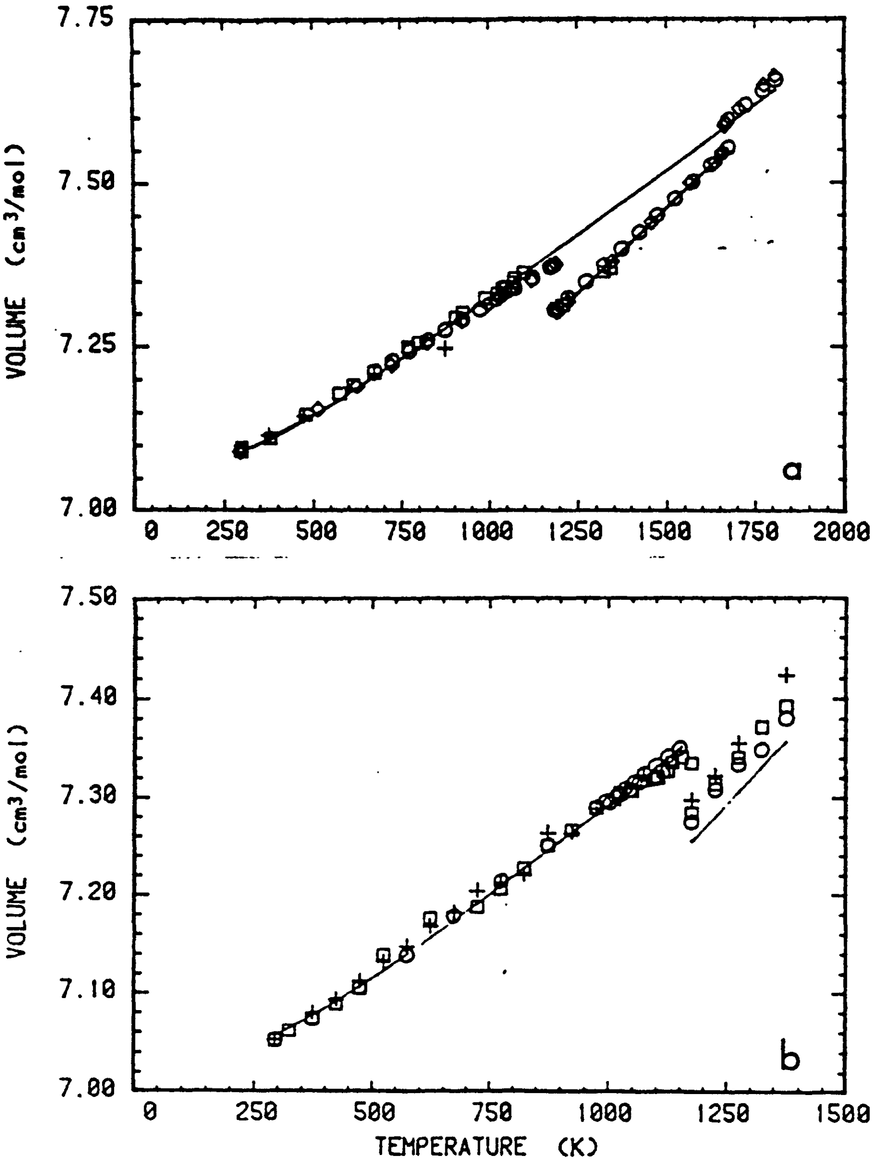

7.75
7.50
7.25
7.00
VOLUME (cm^3/mol)
0
250
500
750
1000
1250
1500
1750
2000
a
7.50
7.40
7.30
7.20
7.10
7.00
VOLUME (cm^3/mol)
0
250
500
750
1000
1250
1500
b
TEMPERATURE (K)

Figure 7.07

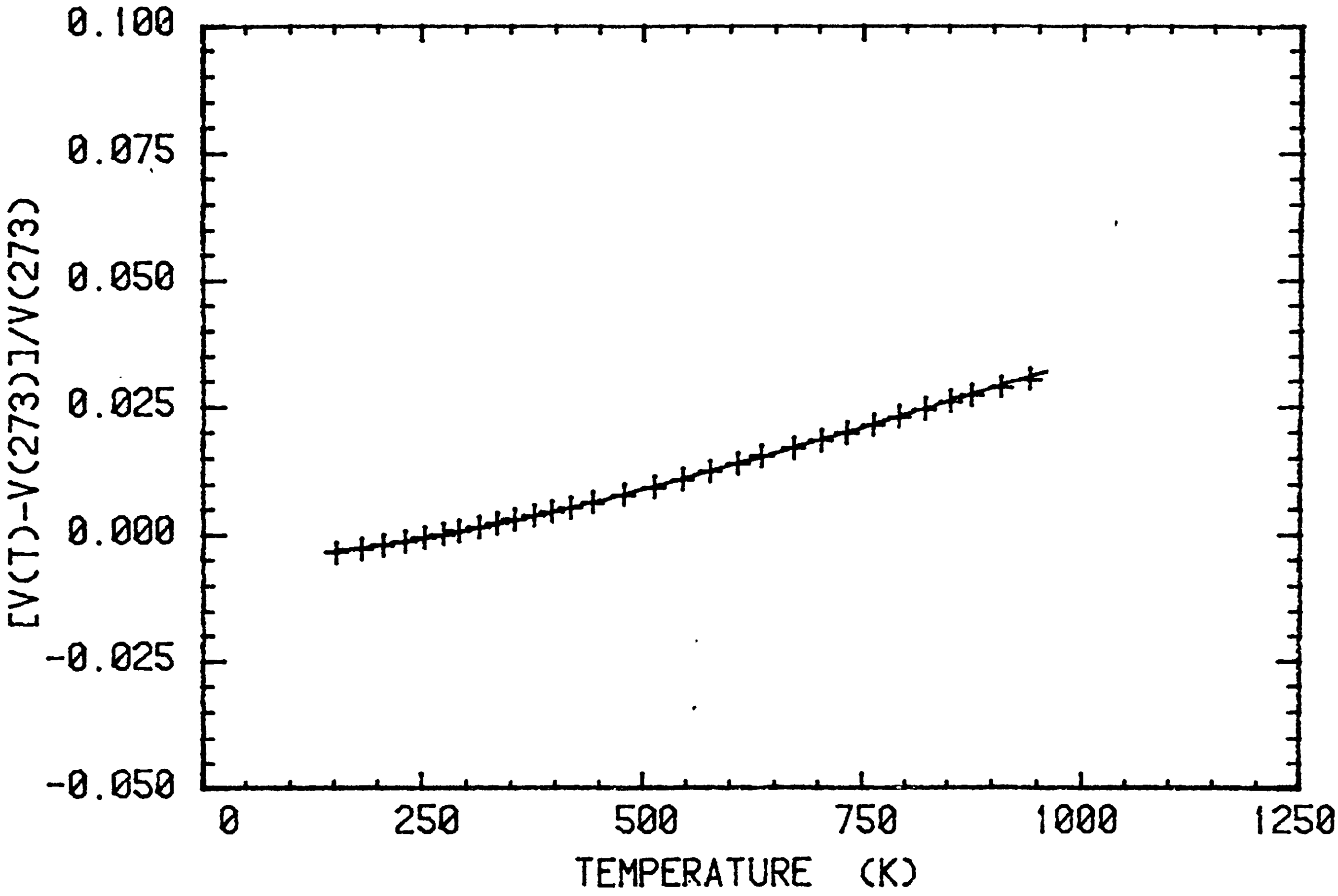
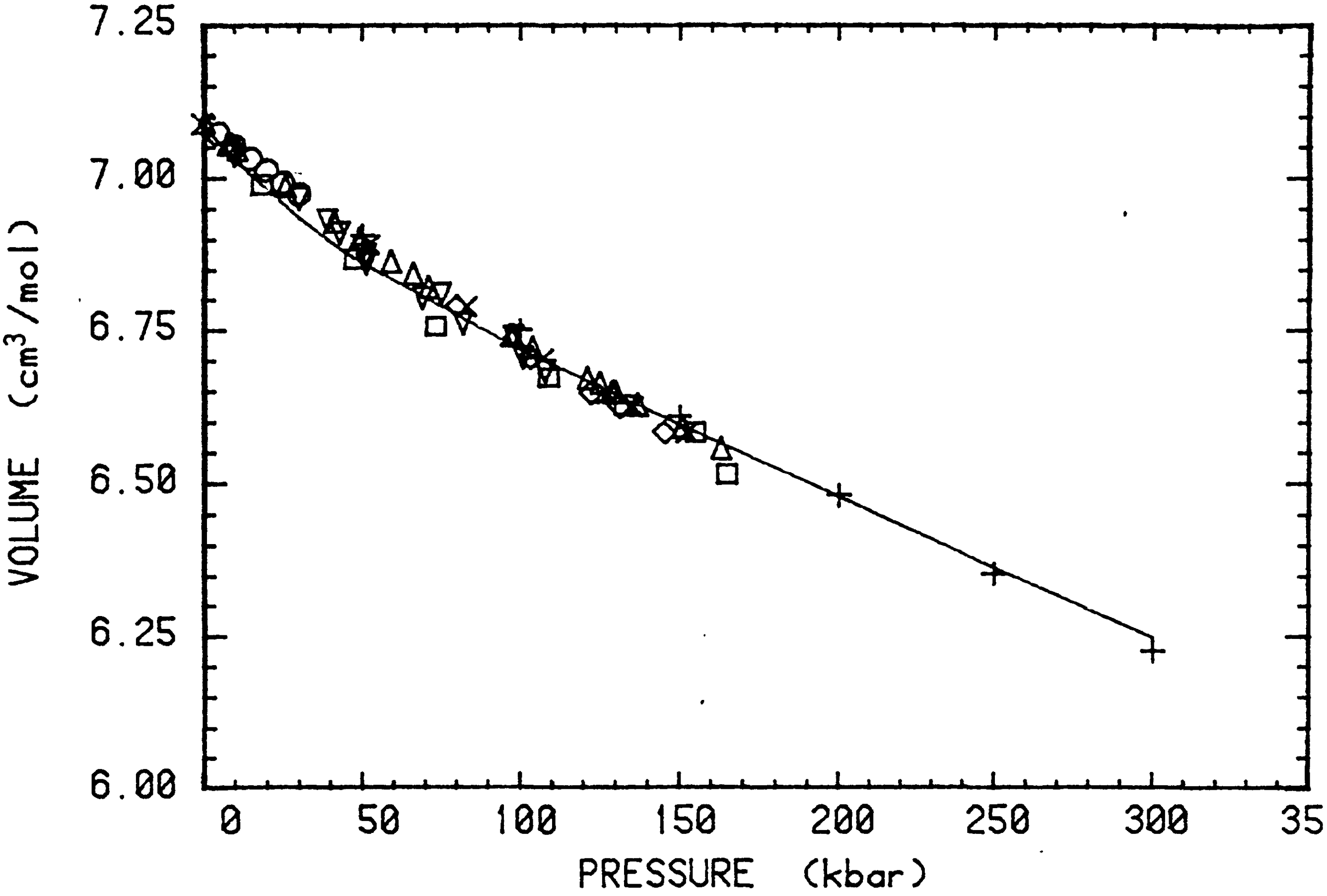

0.100
0.075
0.050
0.025
0.000
-0.025
-0.050
[V(T)-V(273)]/V(273)
0
250
500
750
1000
1250
TEMPERATURE (K)

Figure 7.08



461

Figure 7.89.

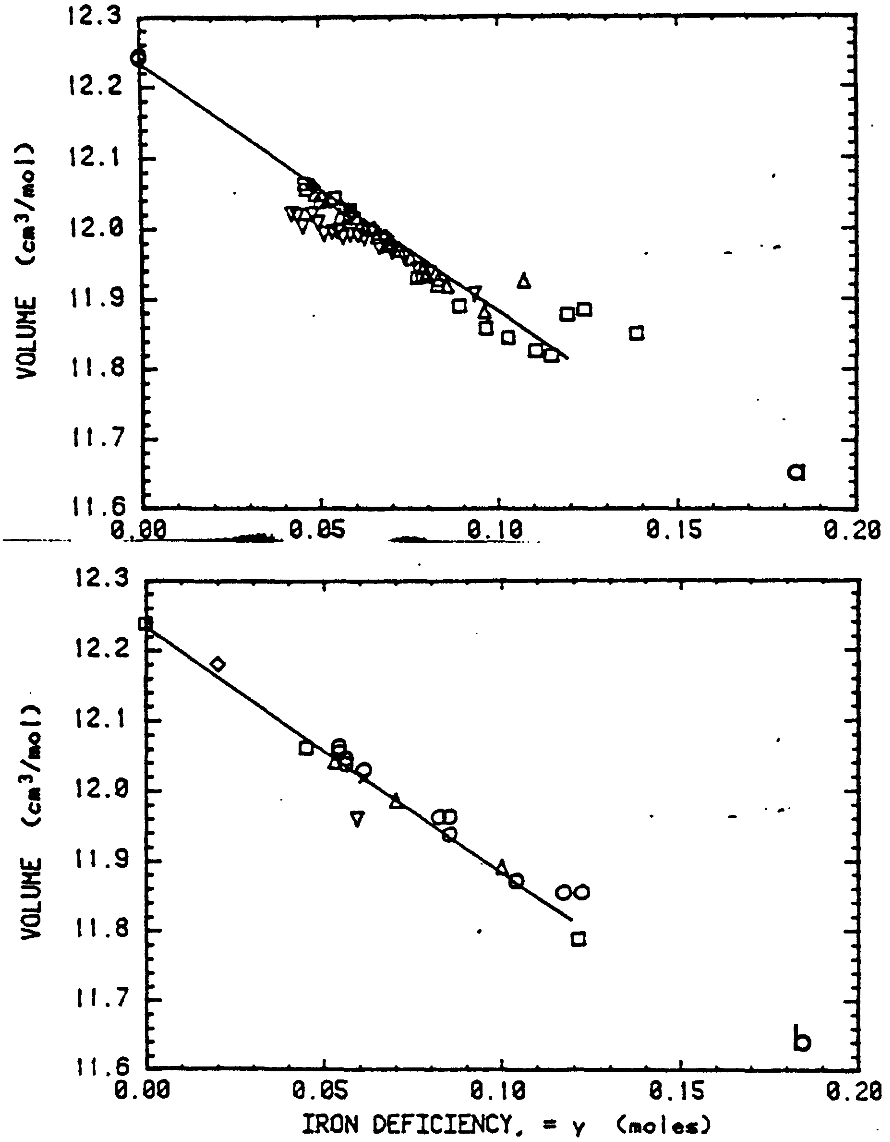


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Figure 7.10

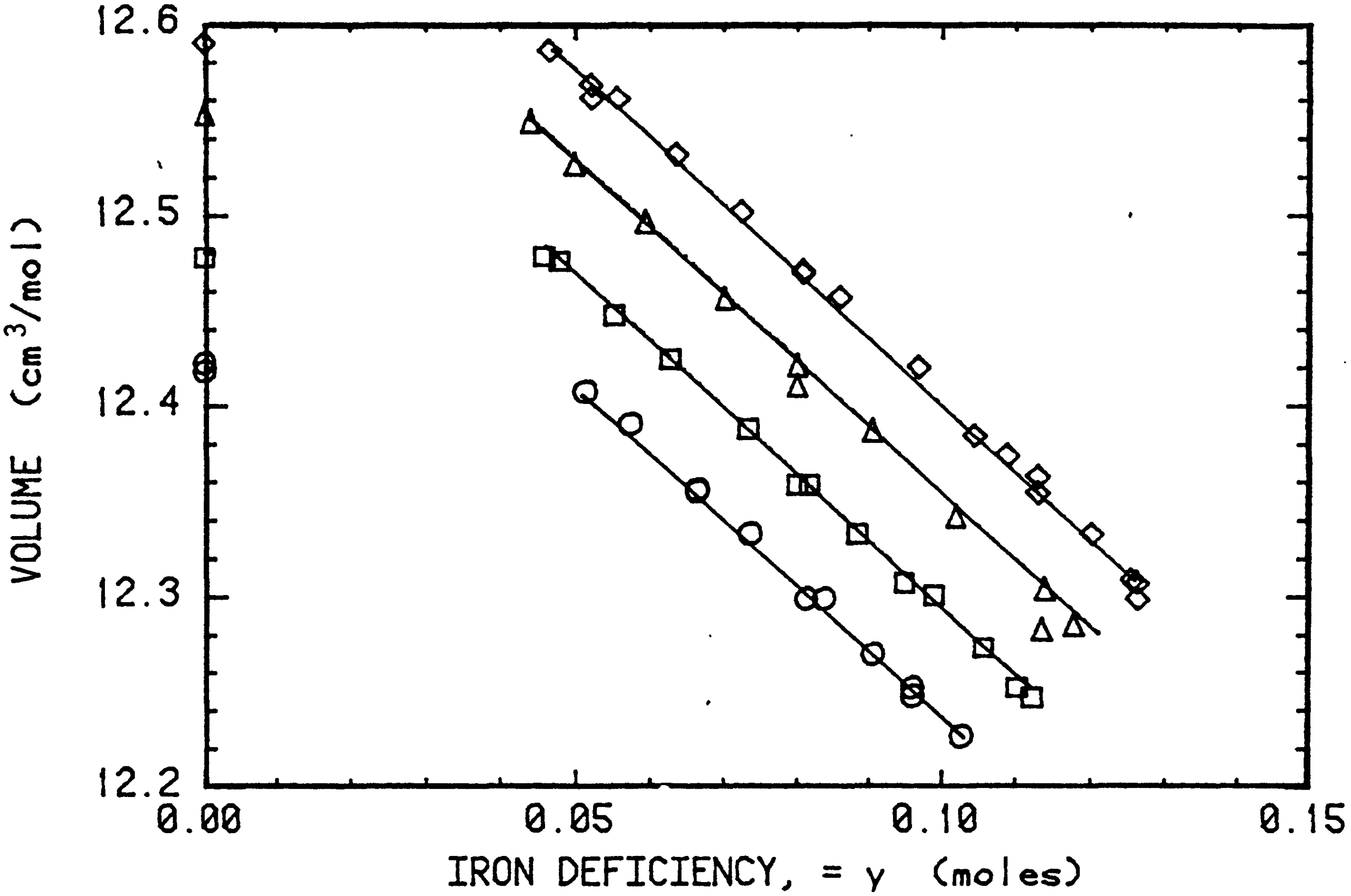
12.6
12.5
12.4
12.3
12.2
VOLUME (cm^3/mol)
0.00
0.05
0.10
0.15
IRON DEFICIENCY, = y (moles)

Figure 7.11.

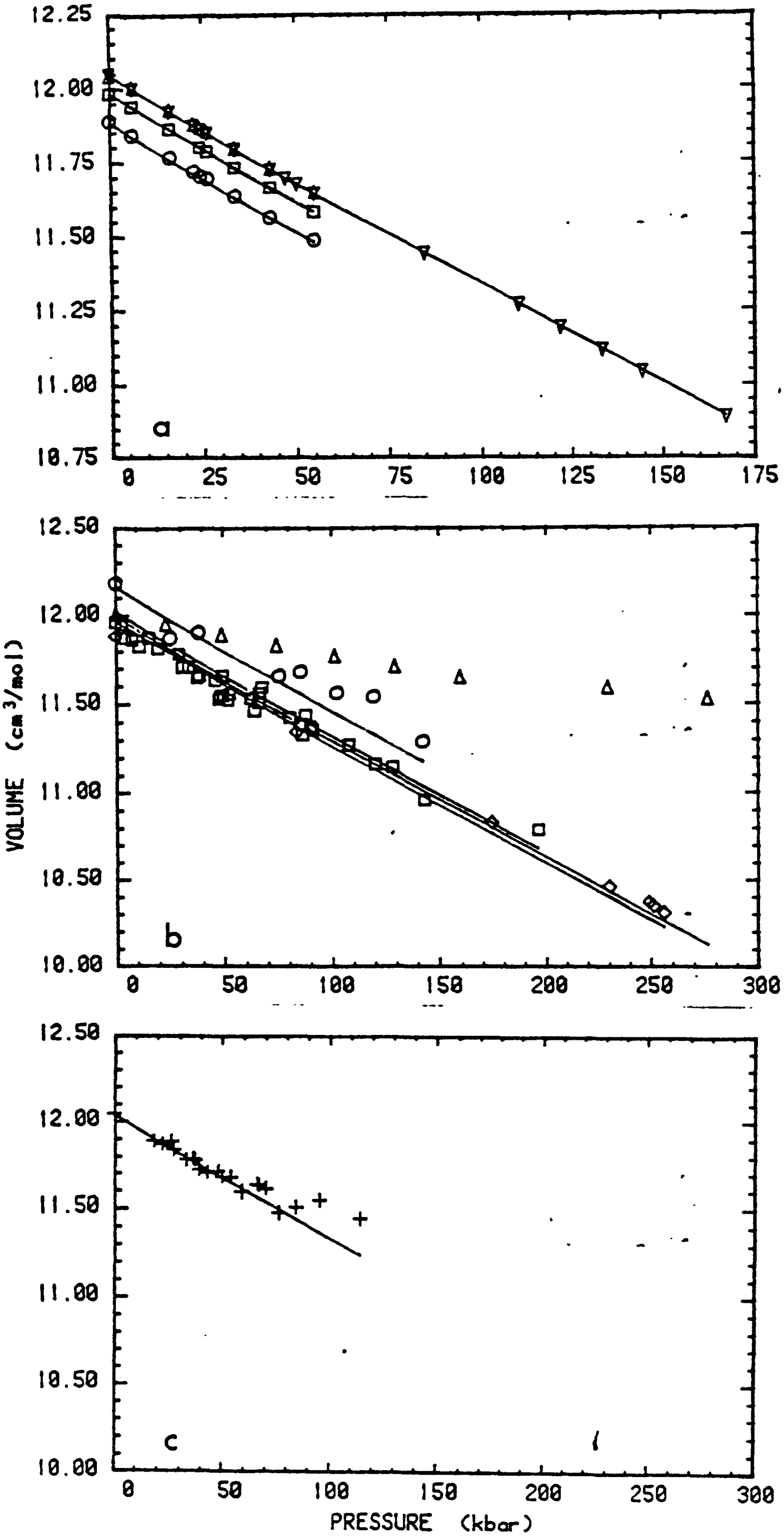

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Figure 7.12

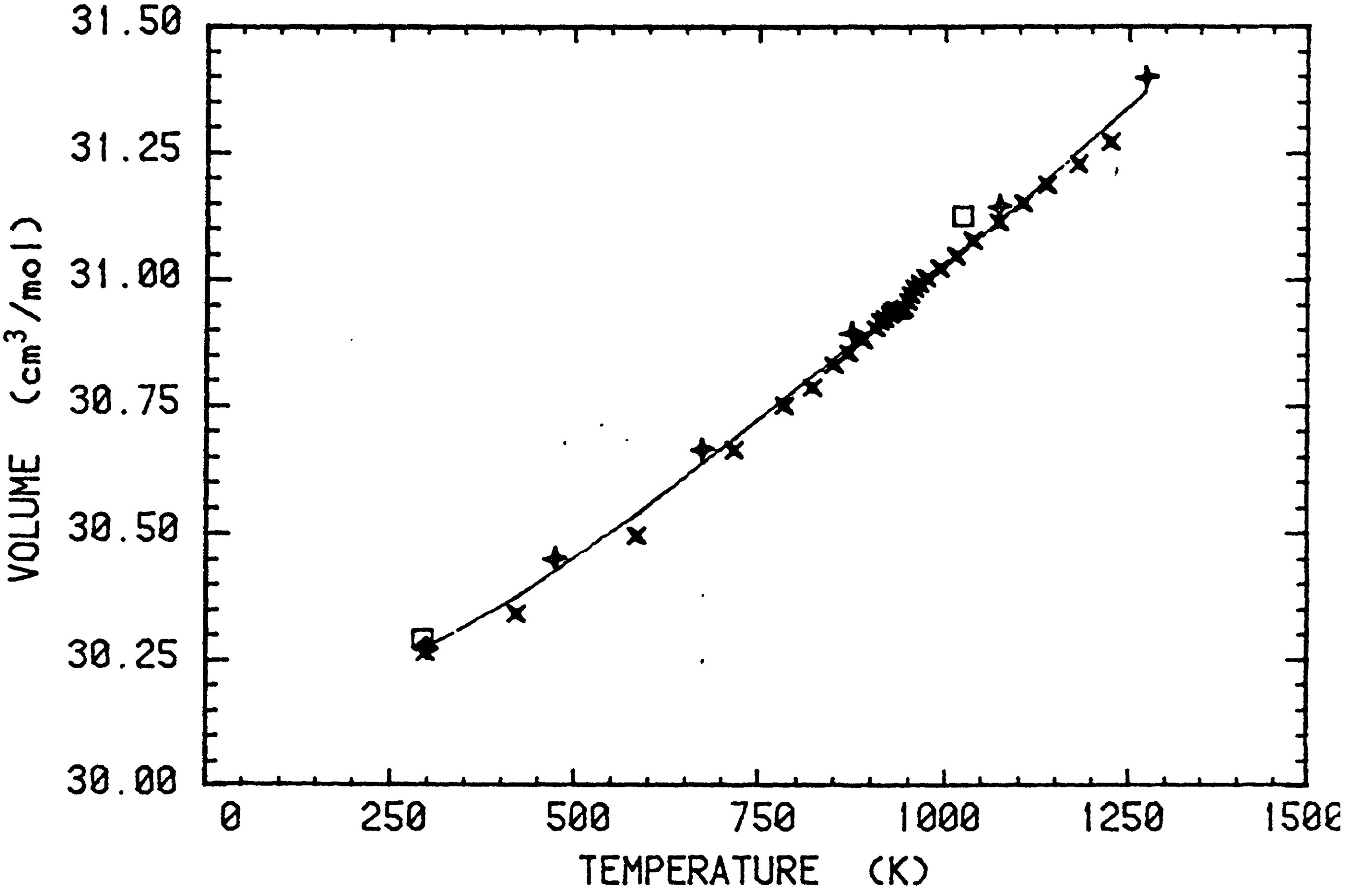

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Figure 7.13

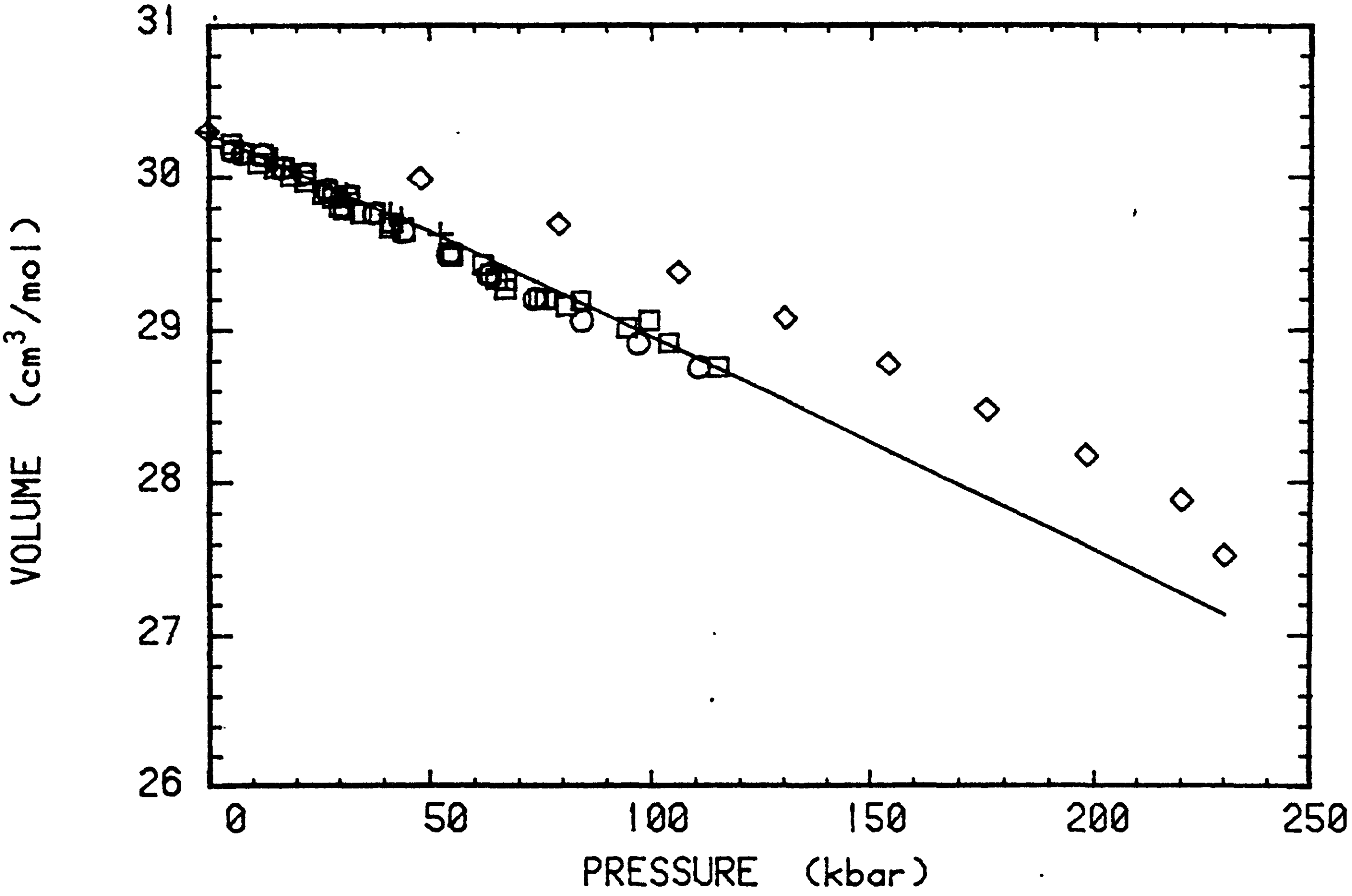
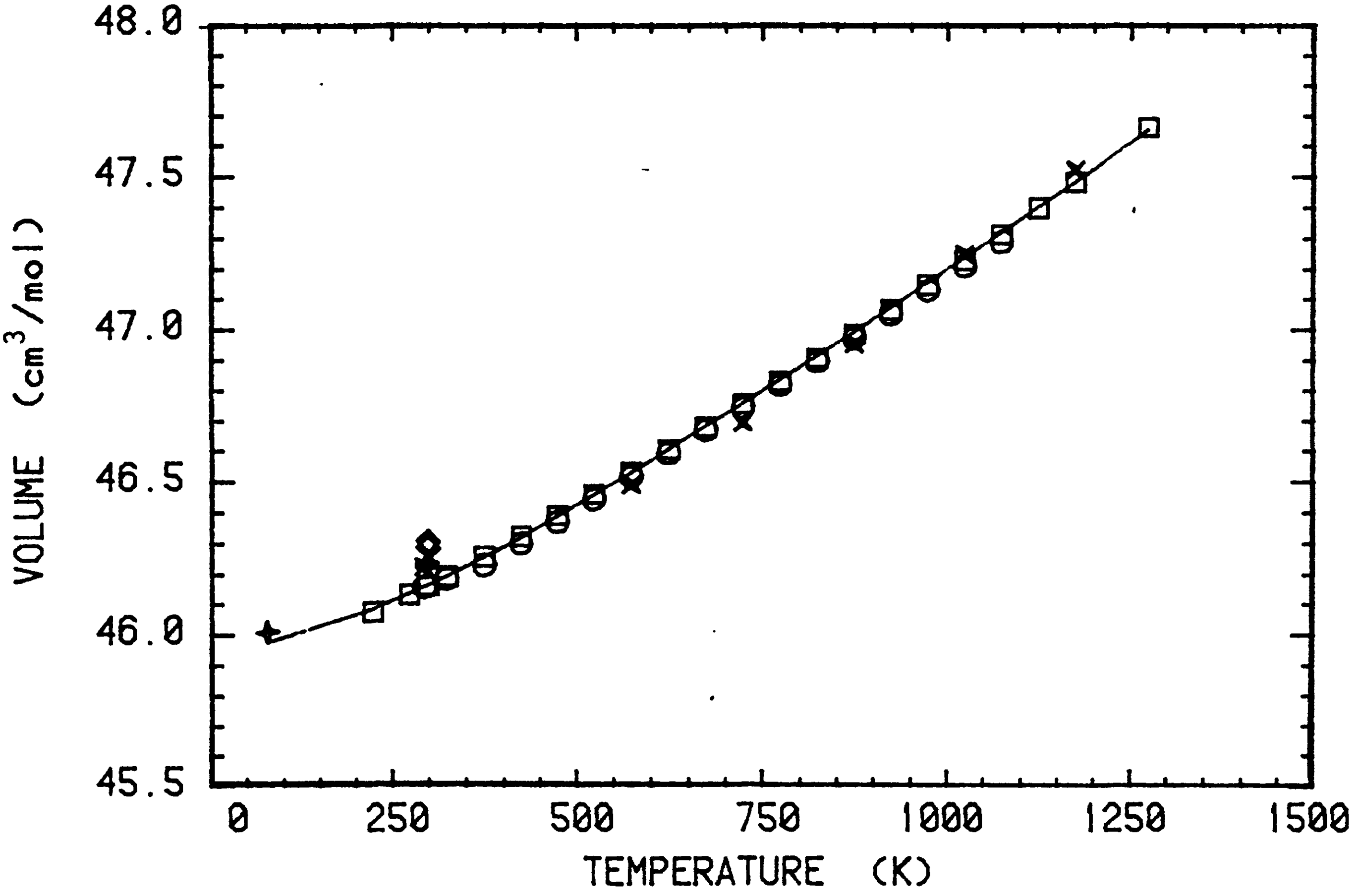


Figure 7.14


48.0
47.5
47.0
46.5
46.0
45.5
VOLUME (cm^3/mol)
0
250
500
750
1000
1250
1500
TEMPERATURE (K)

J.L. Haas, Jr., "Oxygen Buffers" 1-Dec-87

Figure 7.15

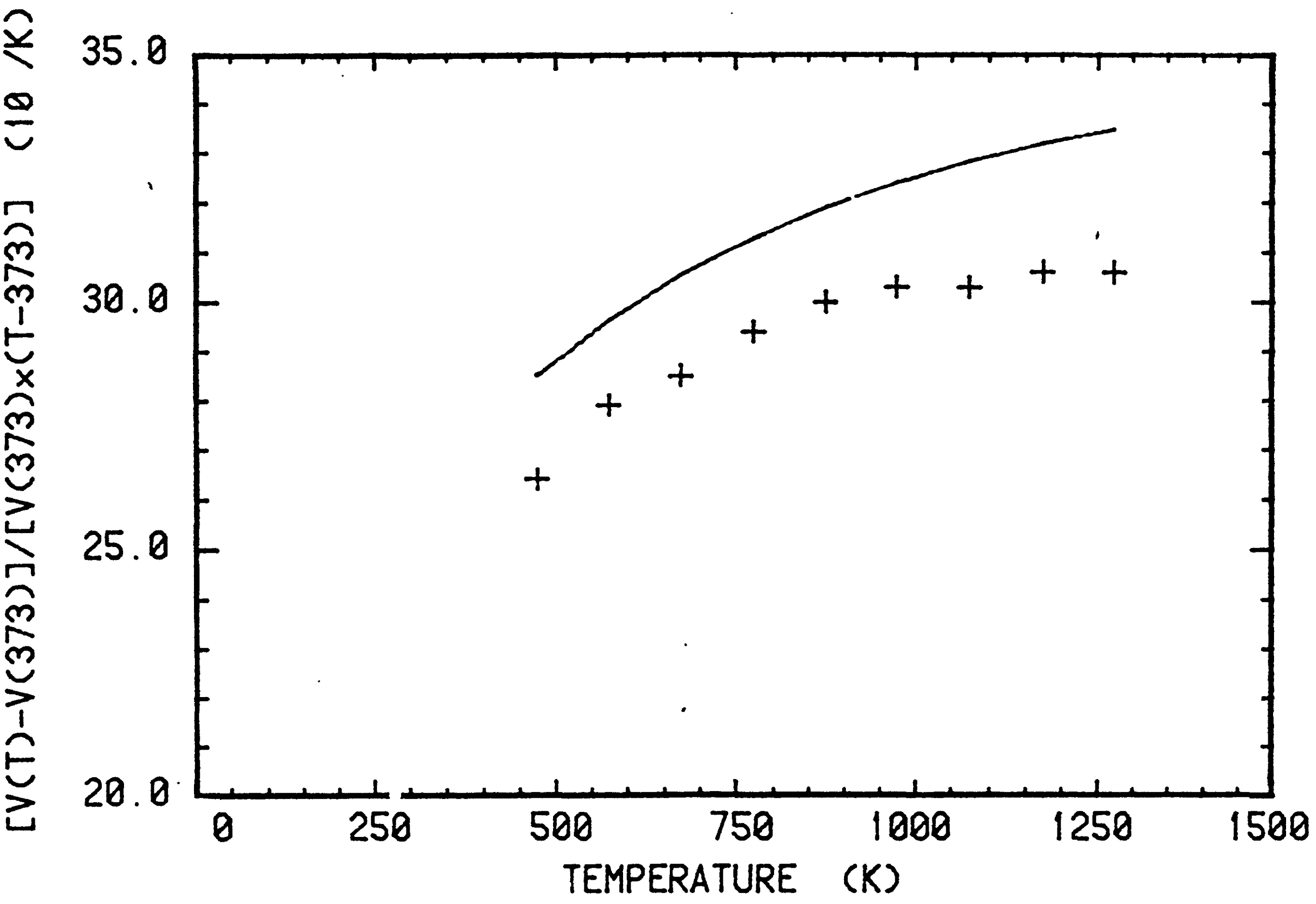


Figure 7.16

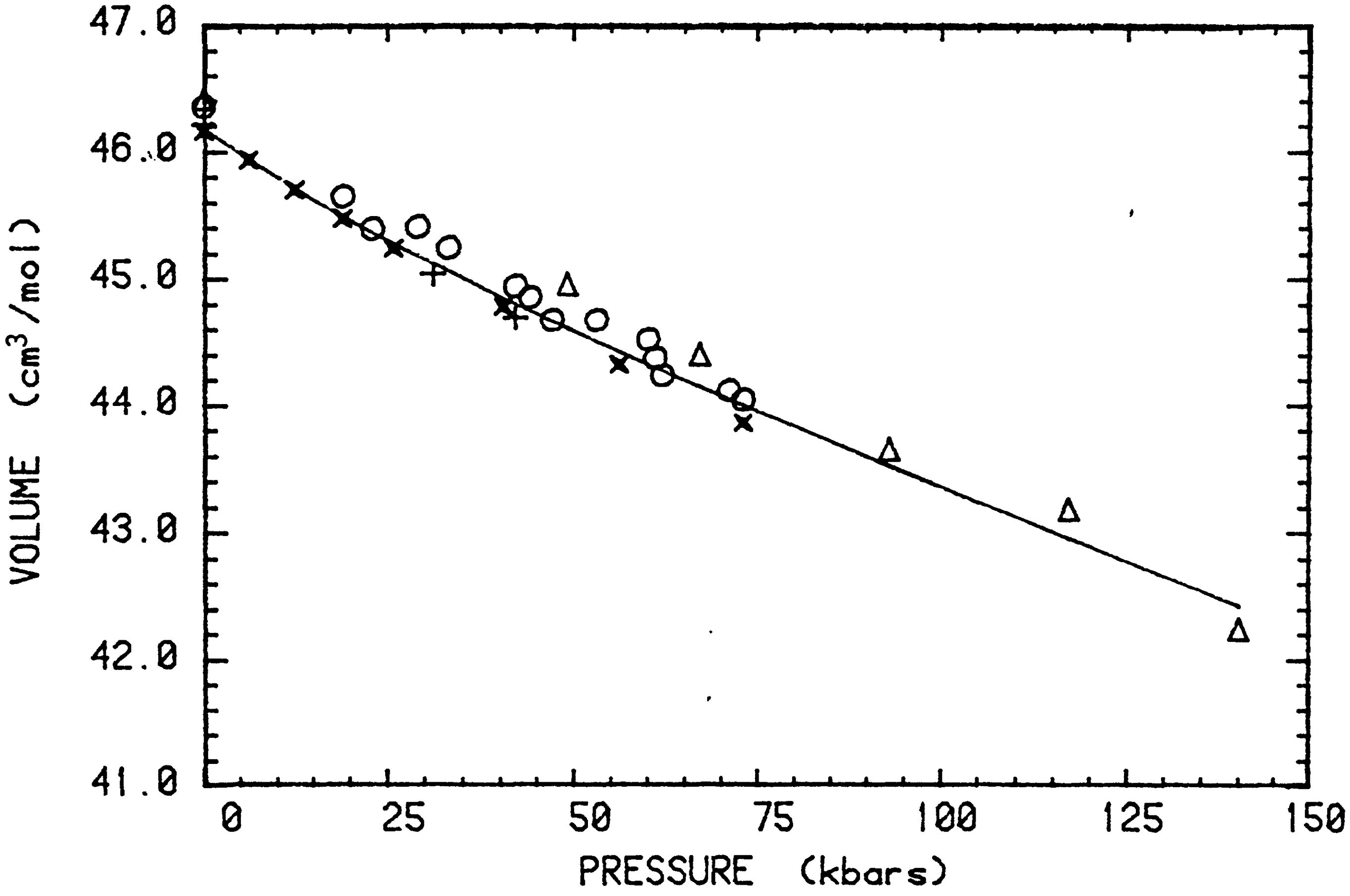

47.0
46.0
45.0
44.0
43.0
42.0
41.0
VOLUME (cm^3/mol)
0
25
50
75
100
125
150
PRESSURE (kbars)

Figure 7.17

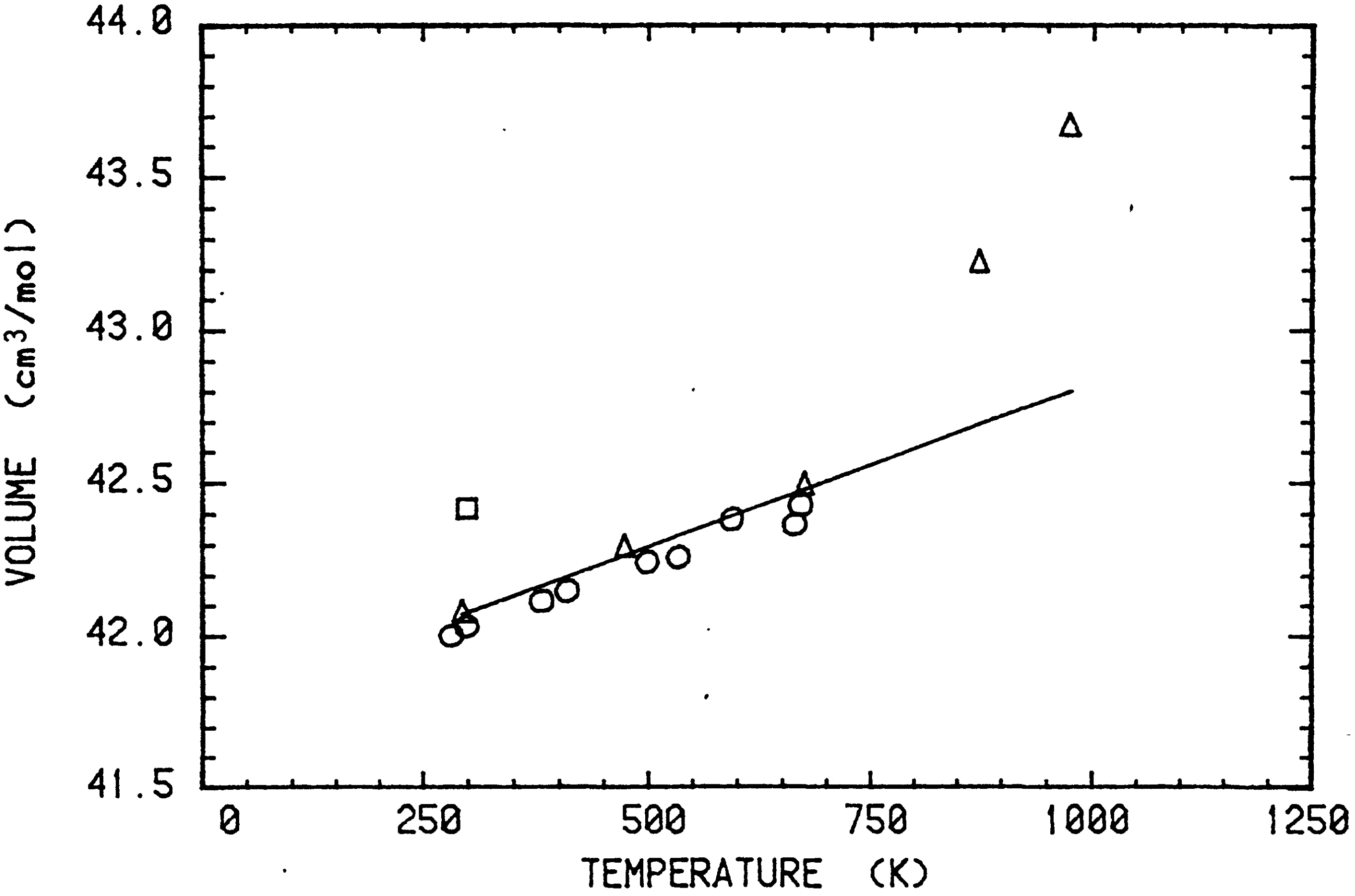

44.0
43.5
43.0
42.5
42.0
41.5
VOLUME (cm3/mol)
0
250
500
750
1000
1250
TEMPERATURE (K)

Figure 7.18

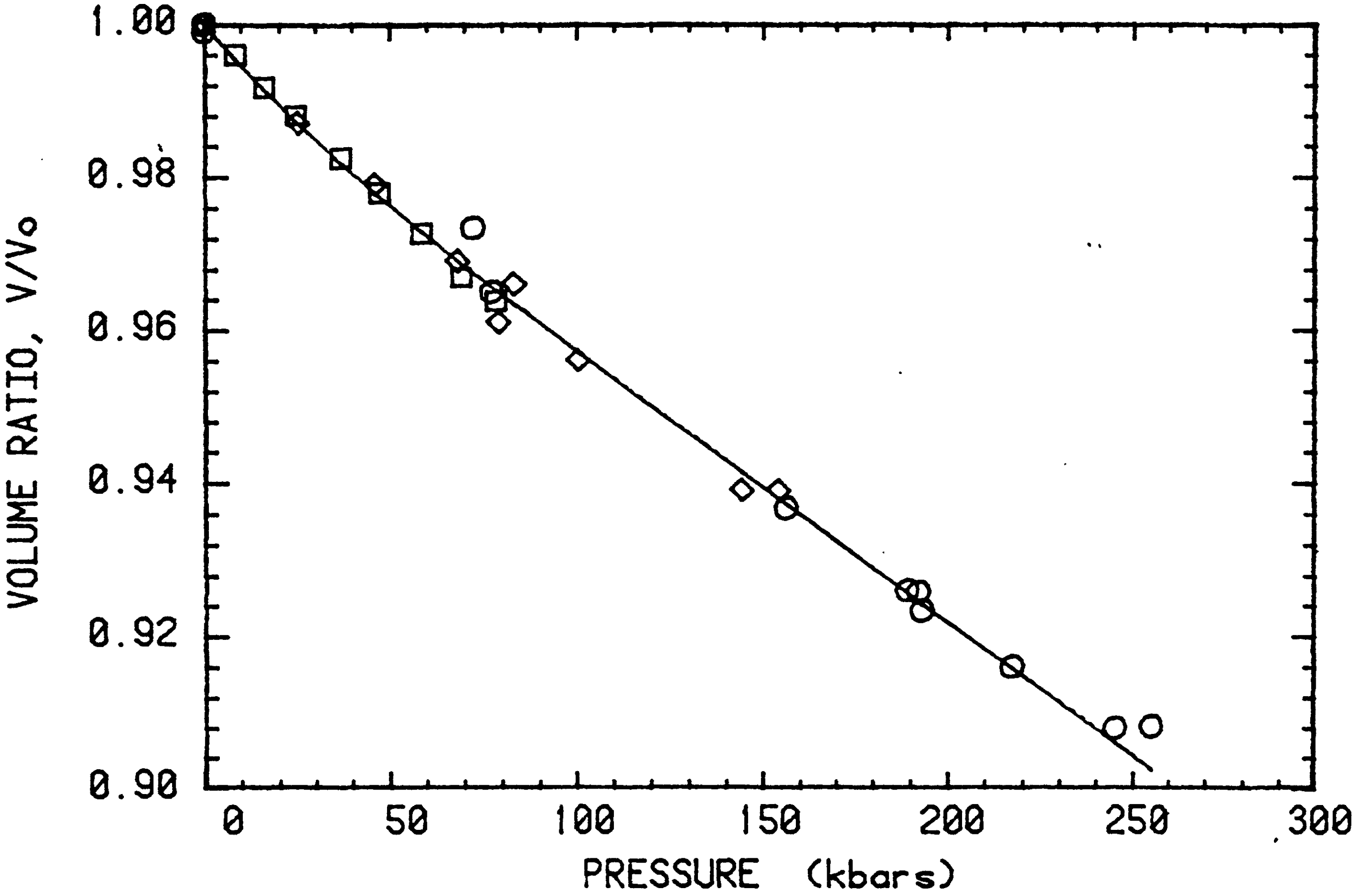

1.00
0.98
0.96
0.94
0.92
0.90
VOLUME RATIO, V/Vo
0
50
100
150
200
250
300
PRESSURE (kbars)

Figure 7.19

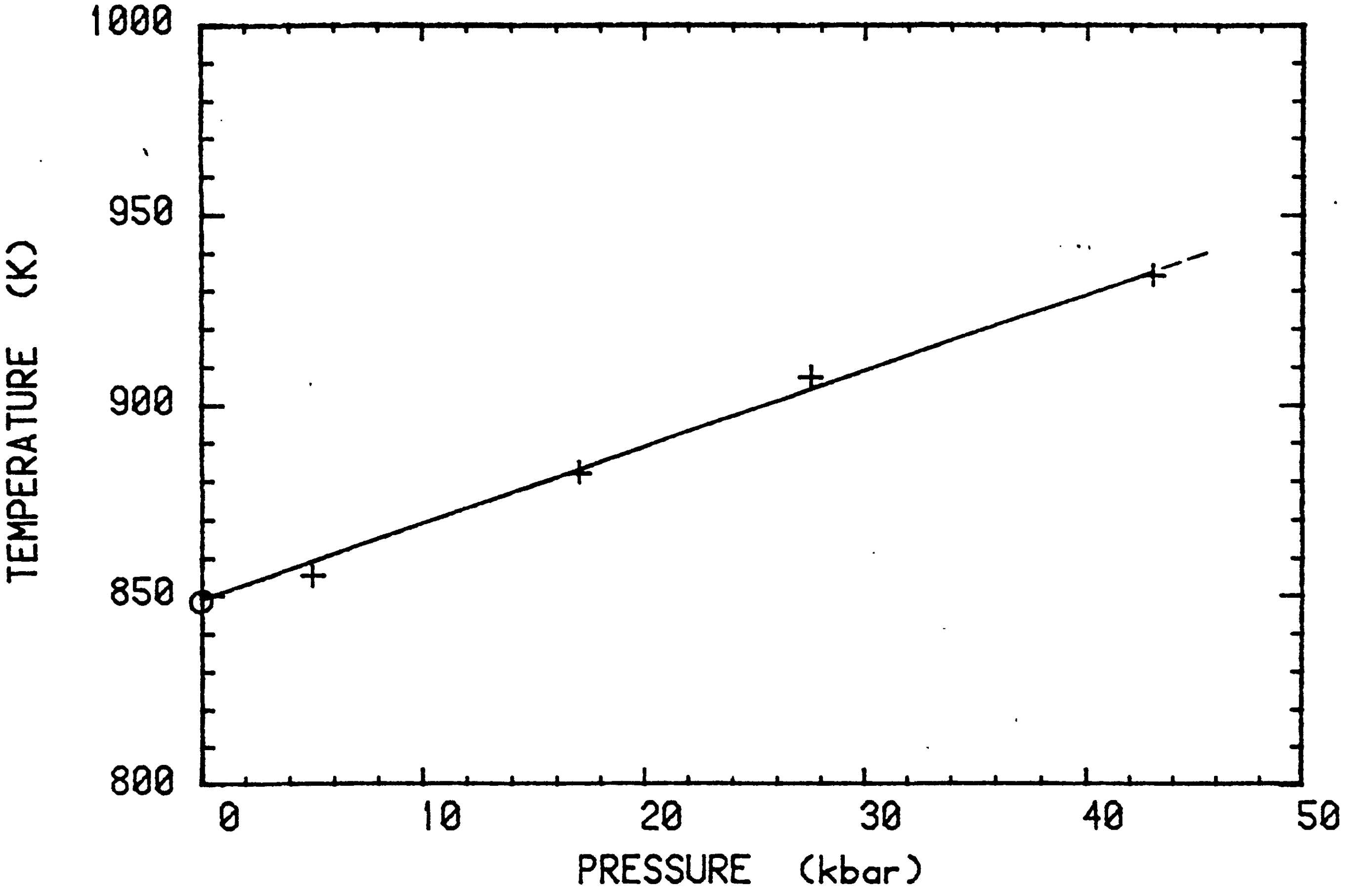

1000
950
900
850
800
TEMPERATURE (K)
0
10
20
30
40
50
PRESSURE (kbar)

Figure 7.20

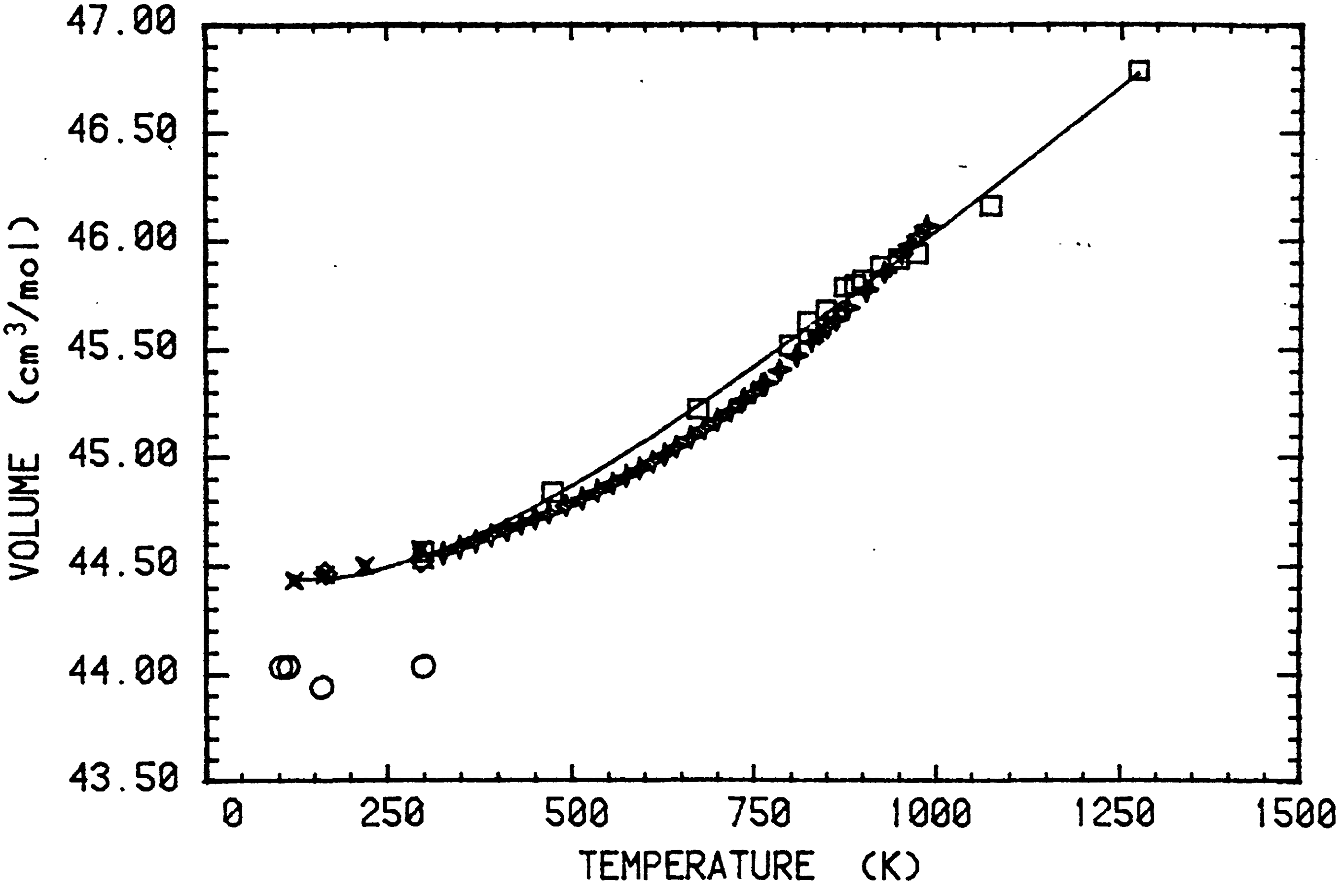

47.00
46.50
46.00
45.50
45.00
44.50
44.00
43.50
VOLUME (cm^3/mol)
0
250
500
750
1000
1250
1500
TEMPERATURE (K)

Figure 7.21

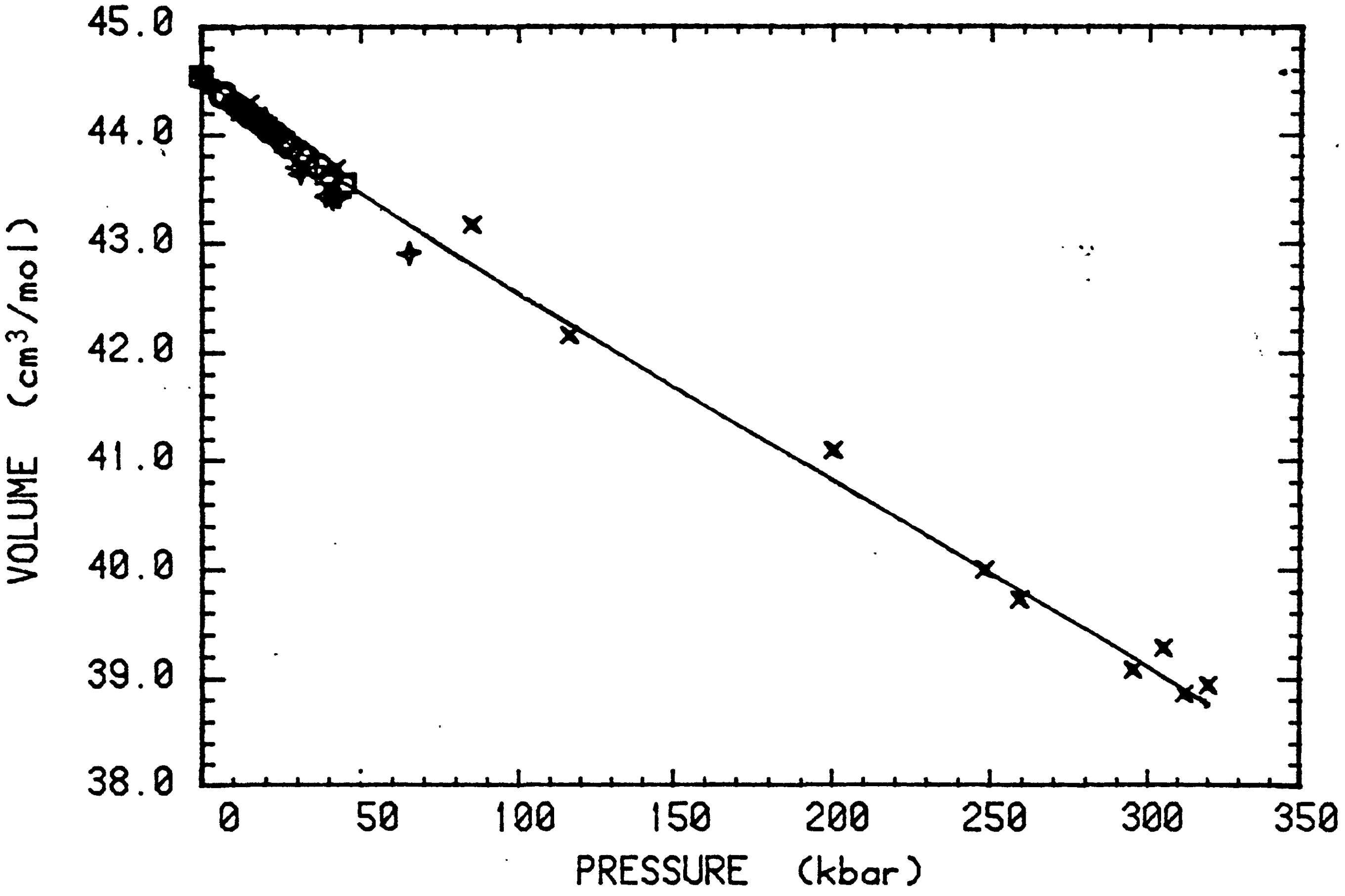
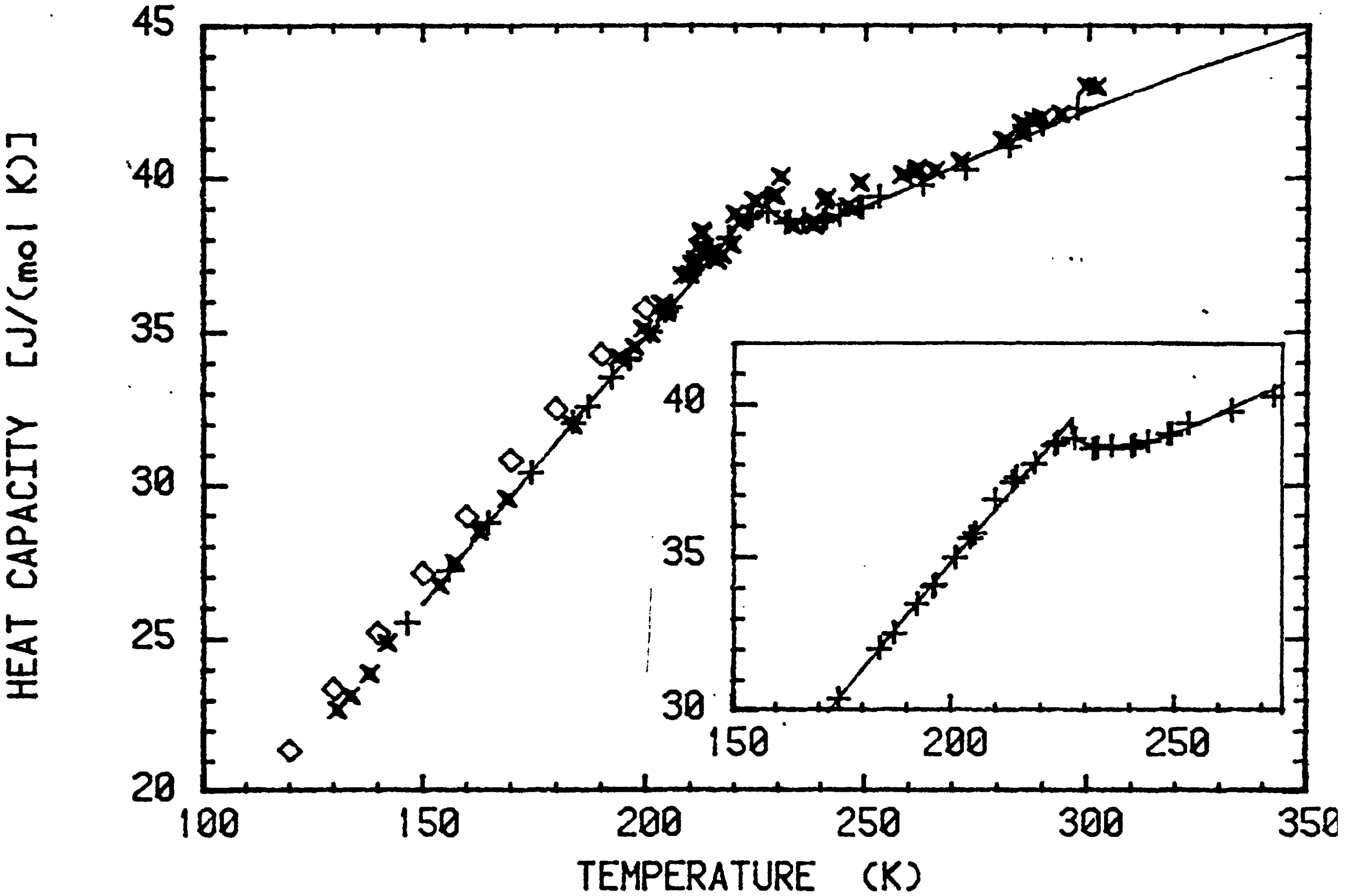

45.0
44.0
43.0
42.0
41.0
40.0
39.0
38.0
VOLUME (cm3/mol)
0
50
100
150
200
250
300
350
PRESSURE (kbar)

Figure 7.22



475

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Figure 7.23

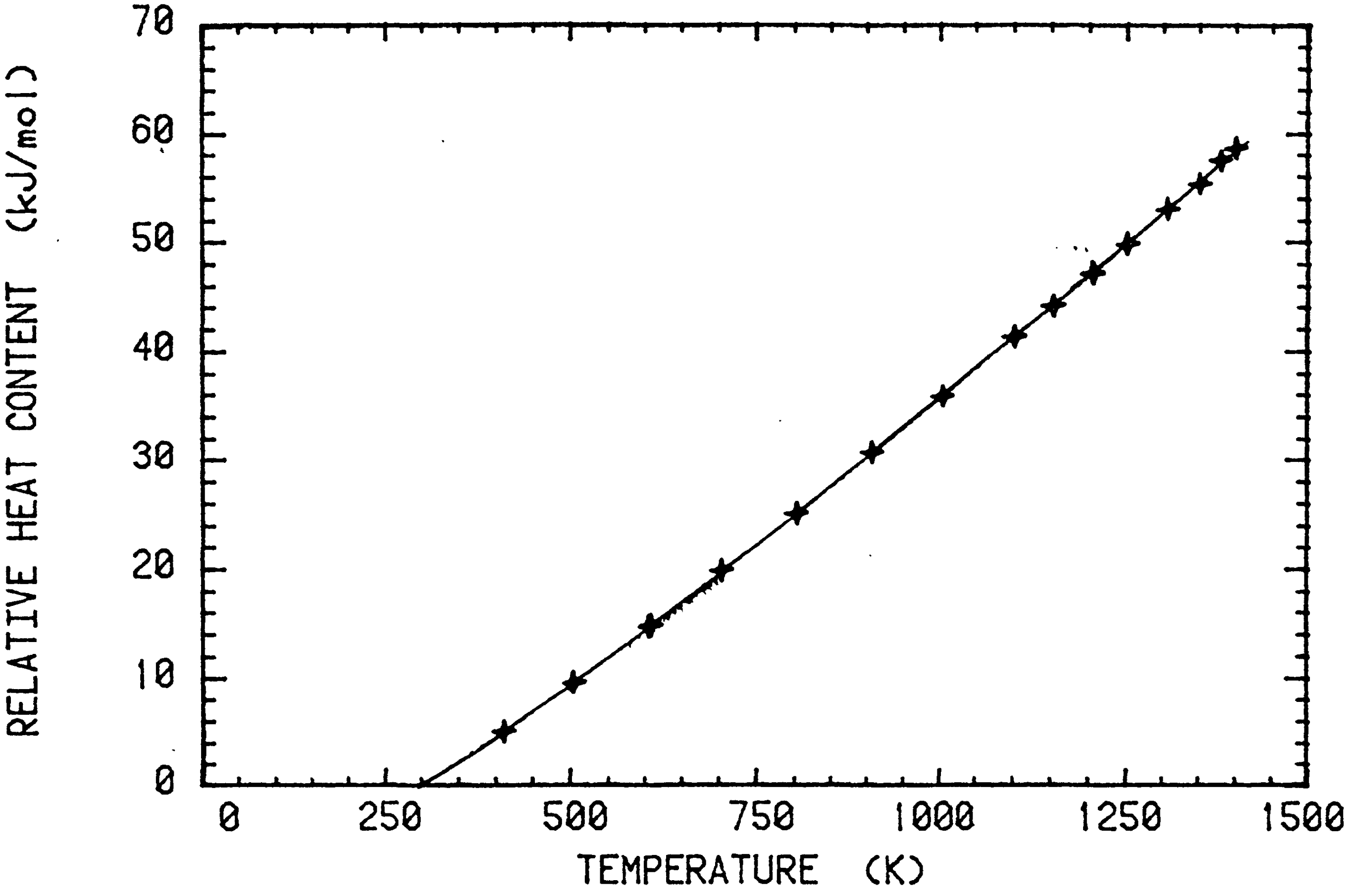

Figure 7.24

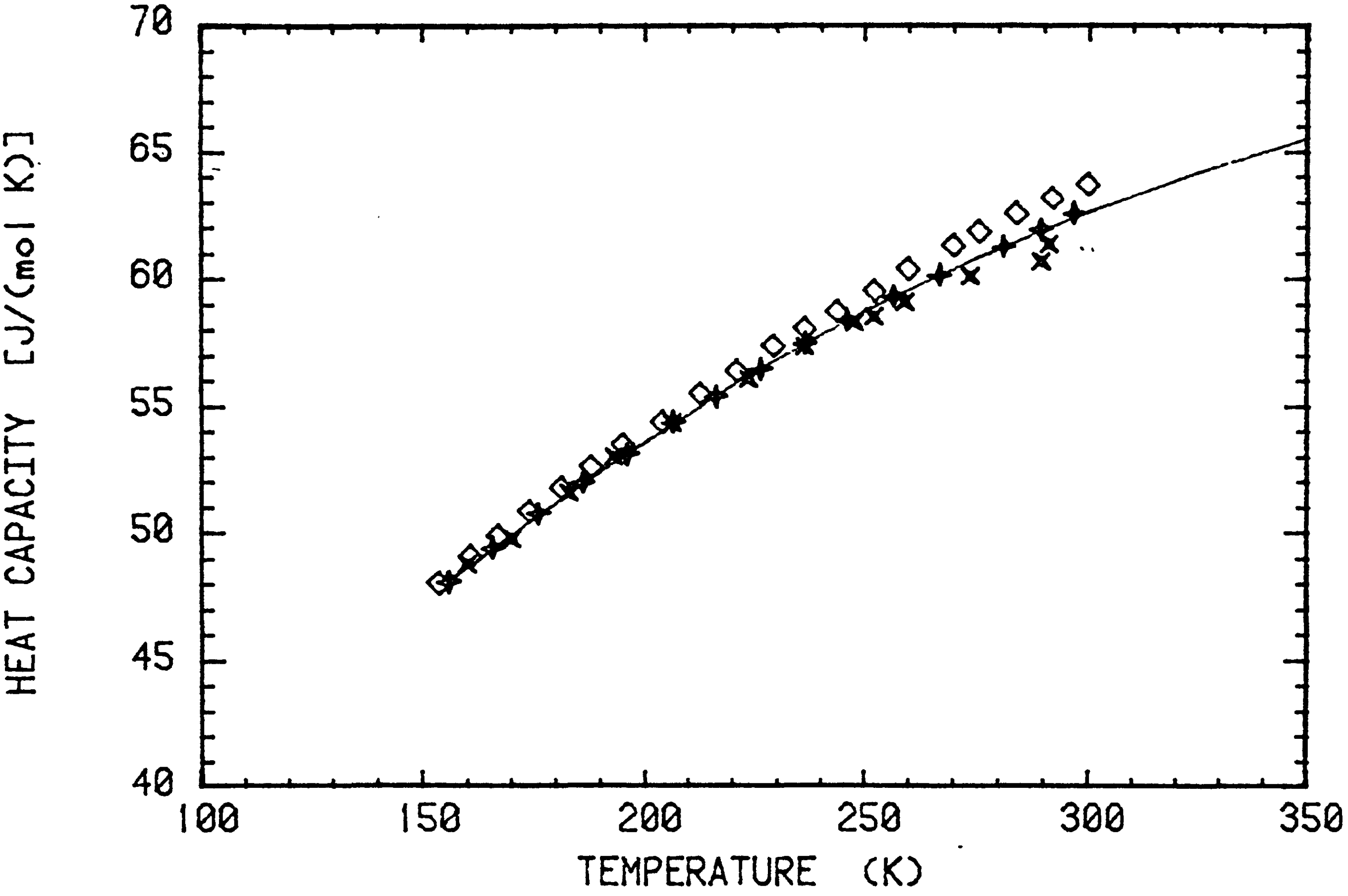
HEAT CAPACITY [J/(mol K)]
70
65
60
55
50
45
40
100
150
200
250
300
350
TEMPERATURE (K)

Figure 7.25

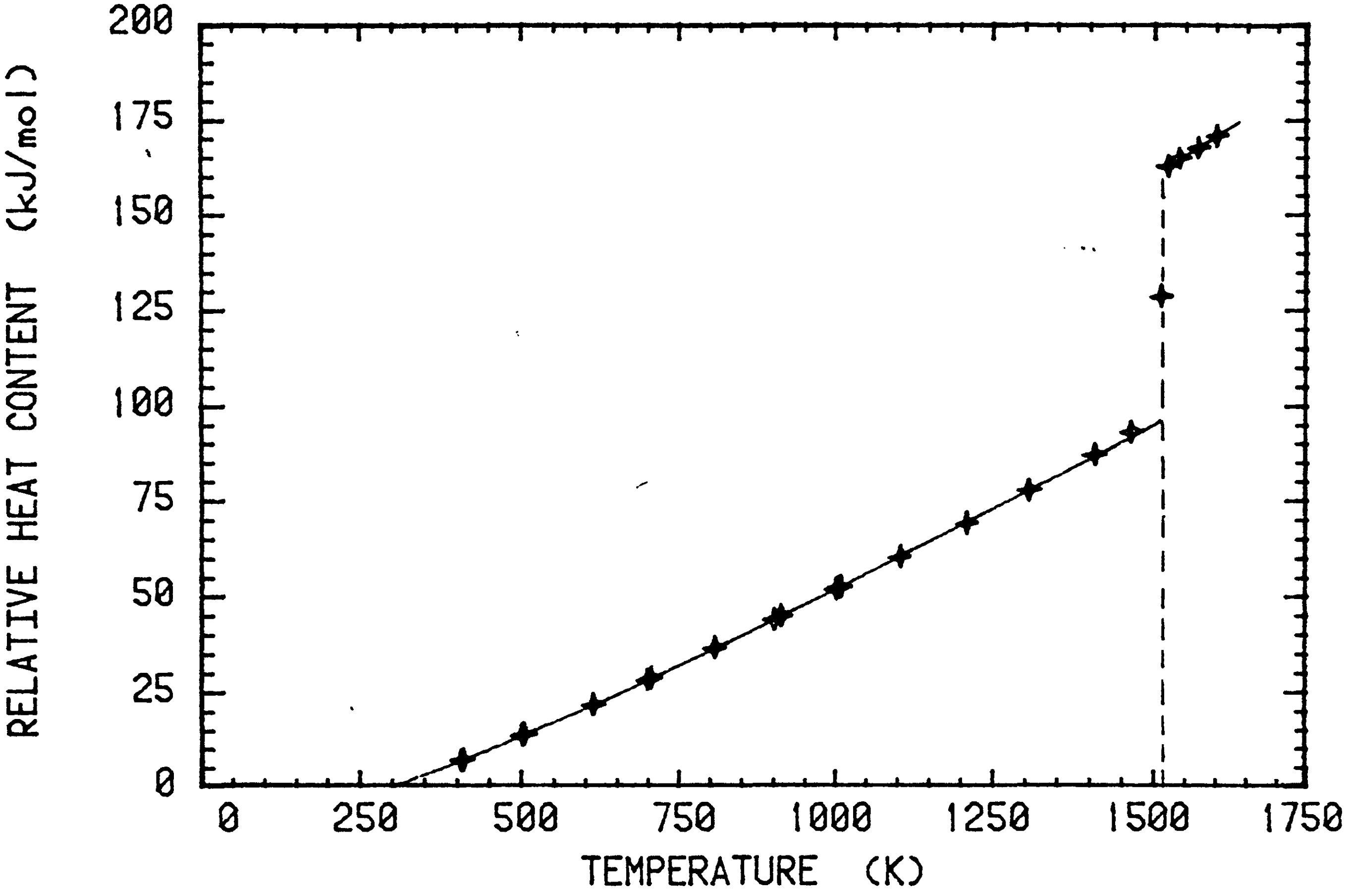
200
175
150
125
100
75
50
25
0
RELATIVE HEAT CONTENT (kJ/mol)
0
250
500
750
1000
1250
1500
1750
TEMPERATURE (K)

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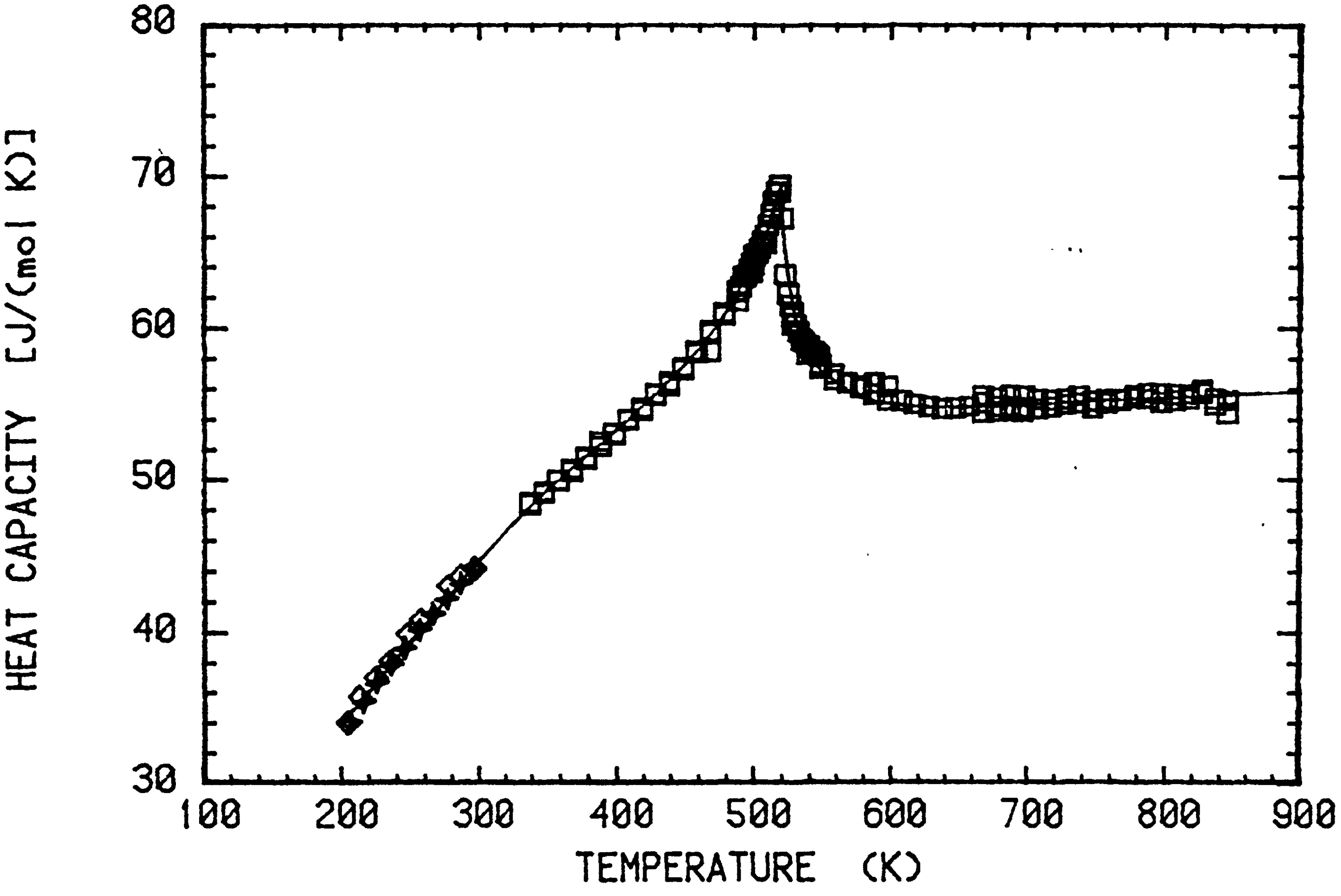
Figure 7.26



479

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Figure 7.27

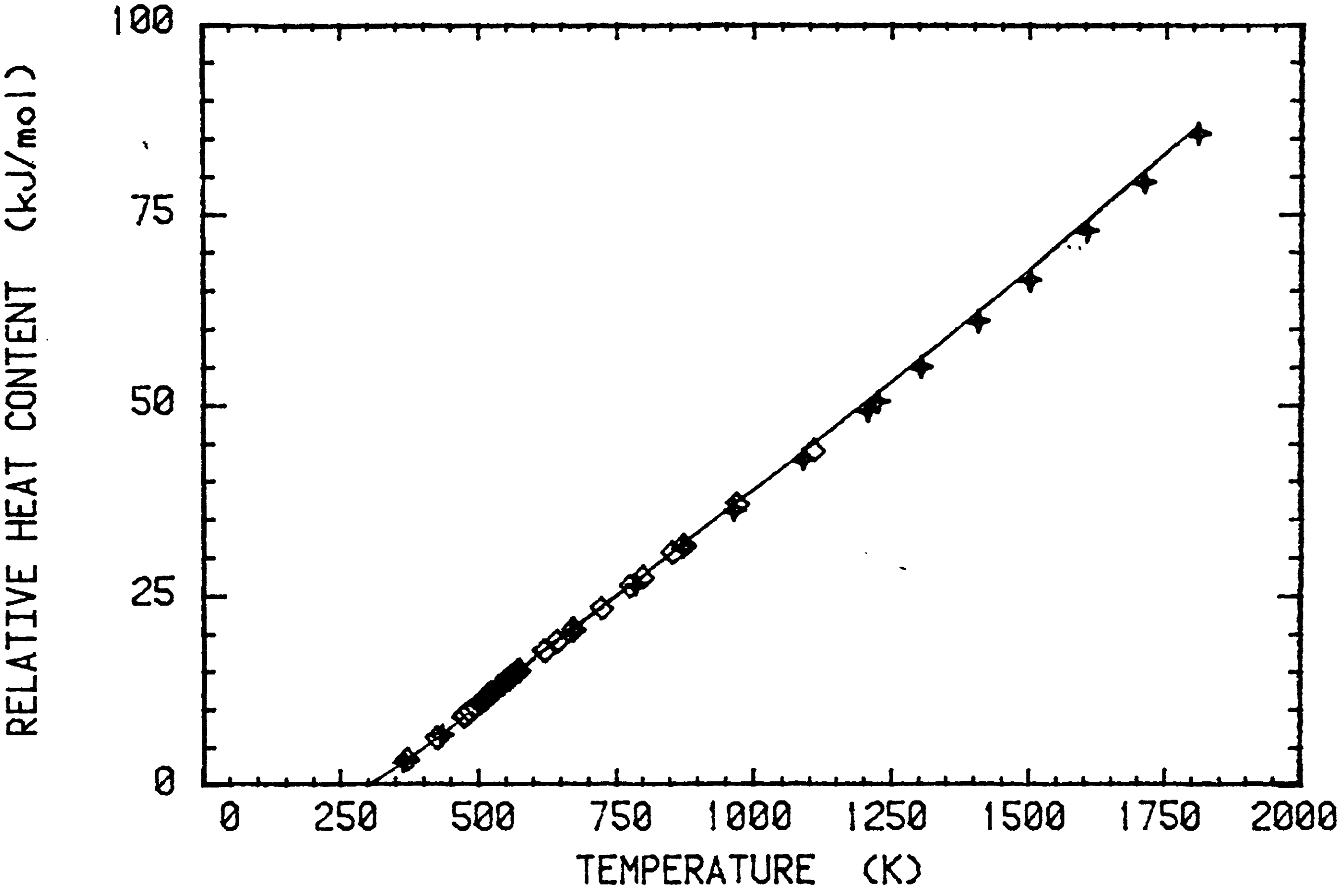
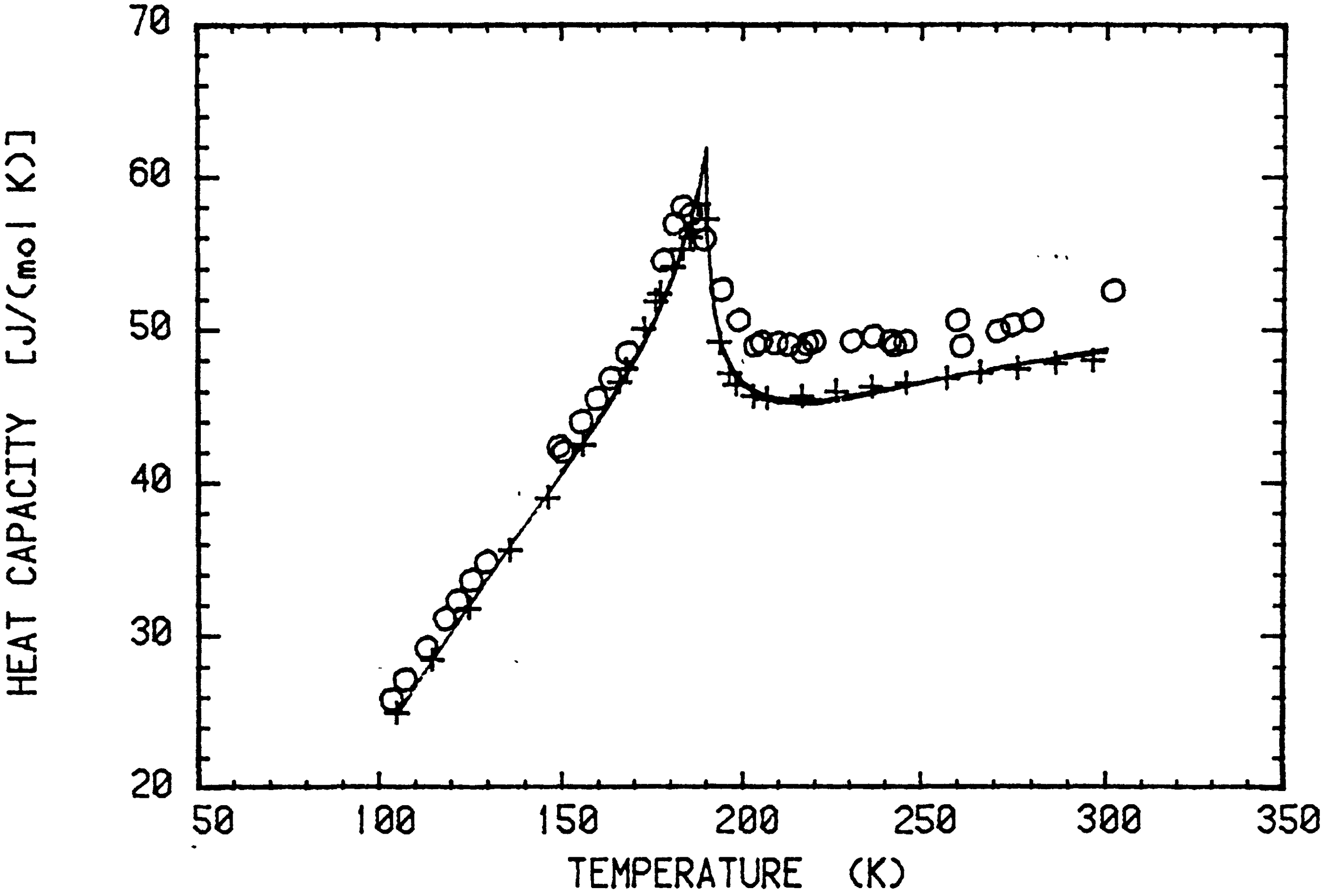
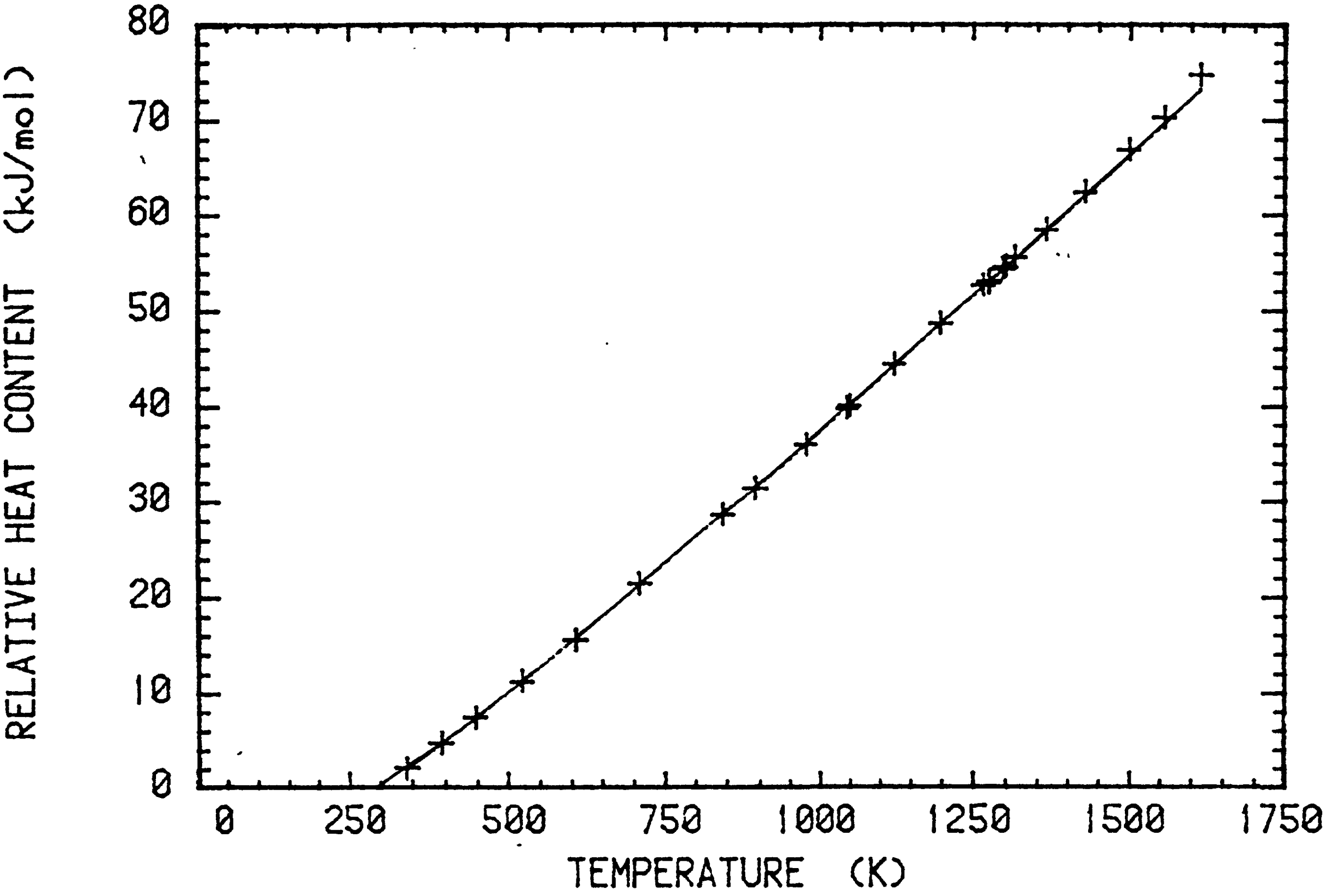


Figure 7.28


HEAT CAPACITY [J/(mol K)]
70
60
50
40
30
20
50
100
150
200
250
300
350
TEMPERATURE (K)

J.L. Haas, Jr., 'Oxygen Buffers' 1-Dec-87

Figure 7.29



482

Figure 7.30

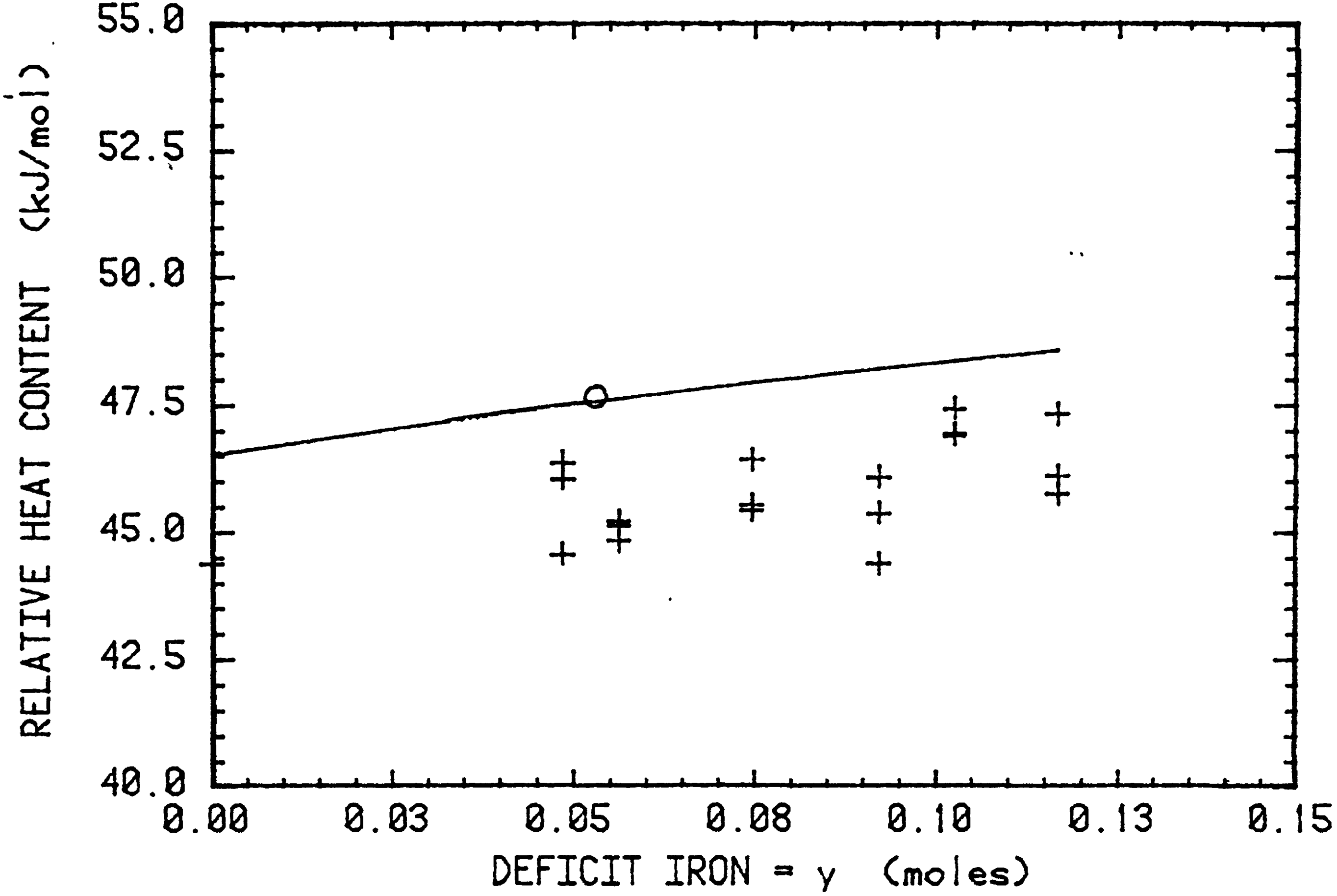

55.0
52.5
50.0
47.5
45.0
42.5
40.0
RELATIVE HEAT CONTENT (kJ/mol)
0.00
0.03
0.05
0.08
0.10
0.13
0.15
DEFICIT IRON = y (moles)

Figure 7.31

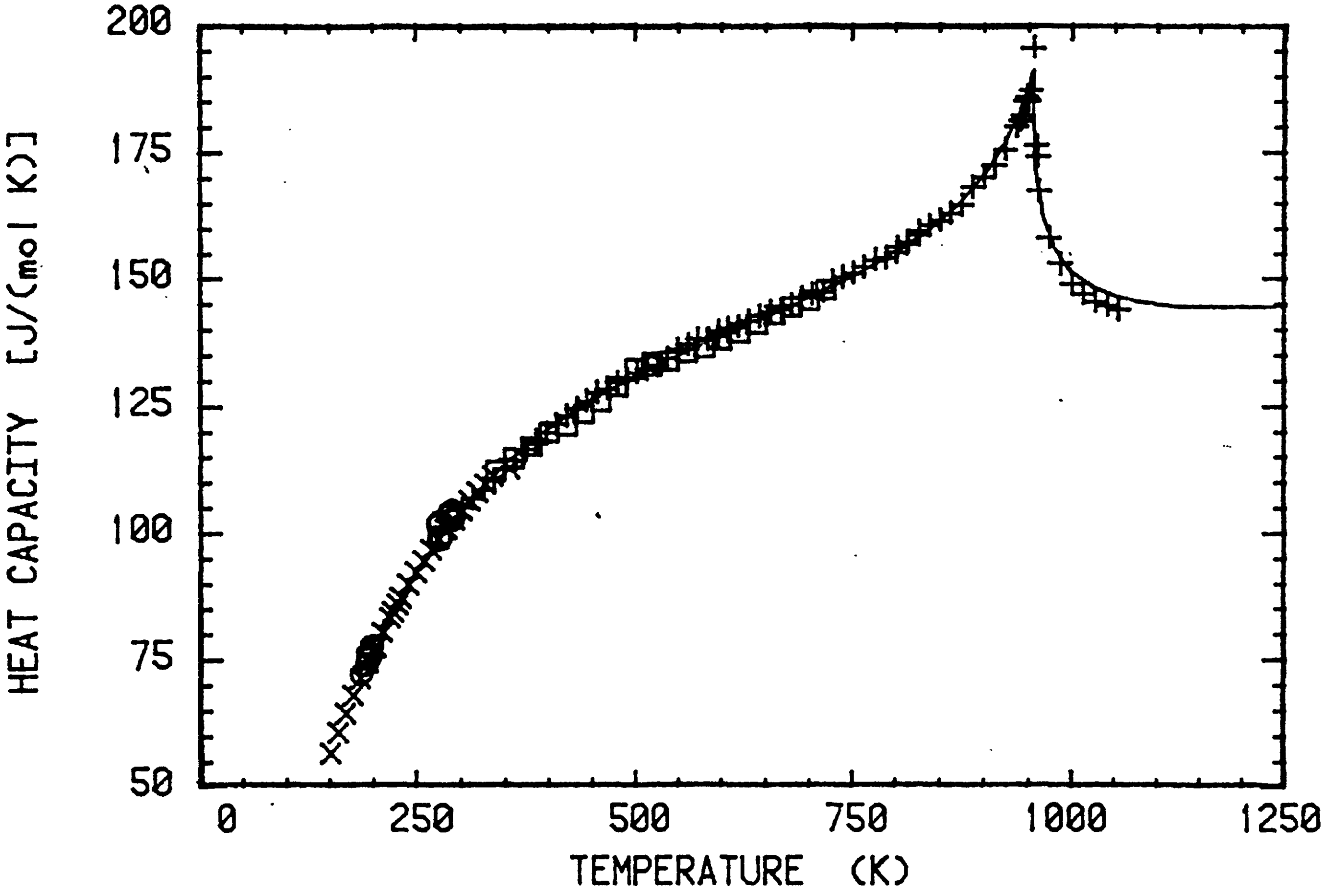
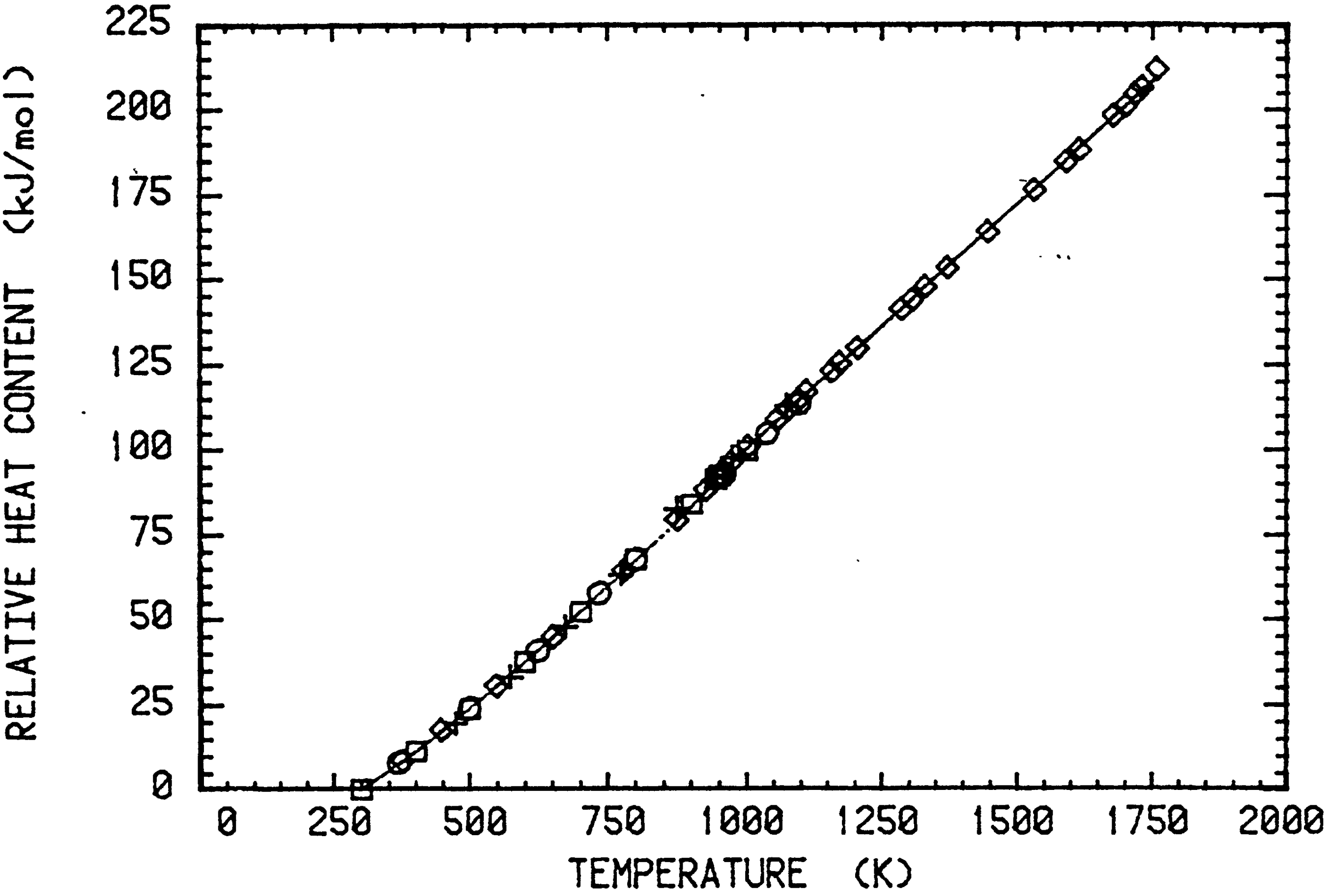

200
175
150
125
100
75
50
0
250
500
750
1000
1250
HEAT CAPACITY [J/(mol K)]
TEMPERATURE (K)

Figure 7.32



RELATIVE HEAT CONTENT (kJ/mol)
225
200
175
150
125
100
75
50
25
0
0
250
500
750
1000
1250
1500
1750
2000
TEMPERATURE (K)

Figure 7.33

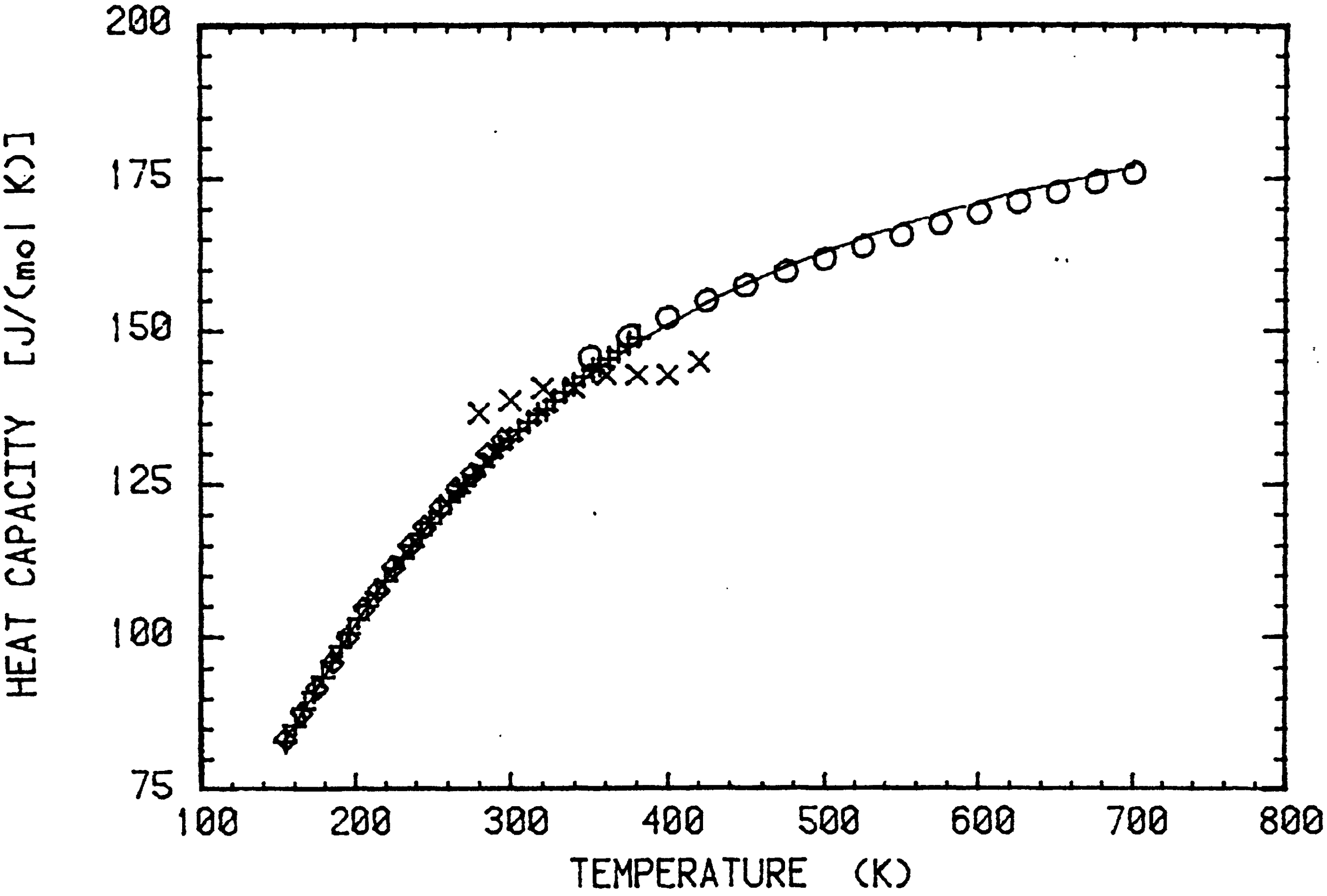

HEAT CAPACITY [J/(mol K)]
200
175
150
125
100
75
100
200
300
400
500
600
700
800
TEMPERATURE (K)

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Figure 7.34

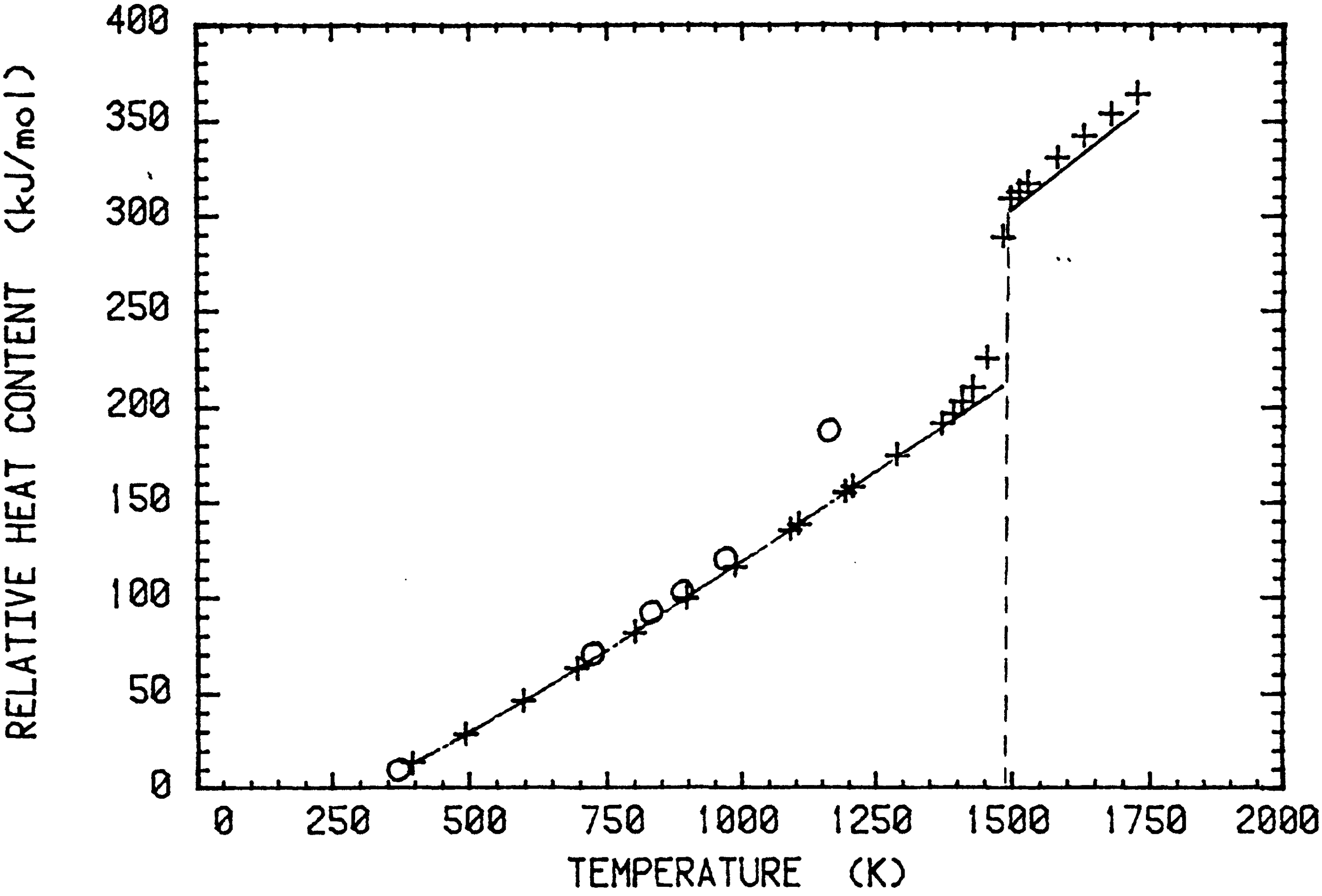

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Figure 7.35

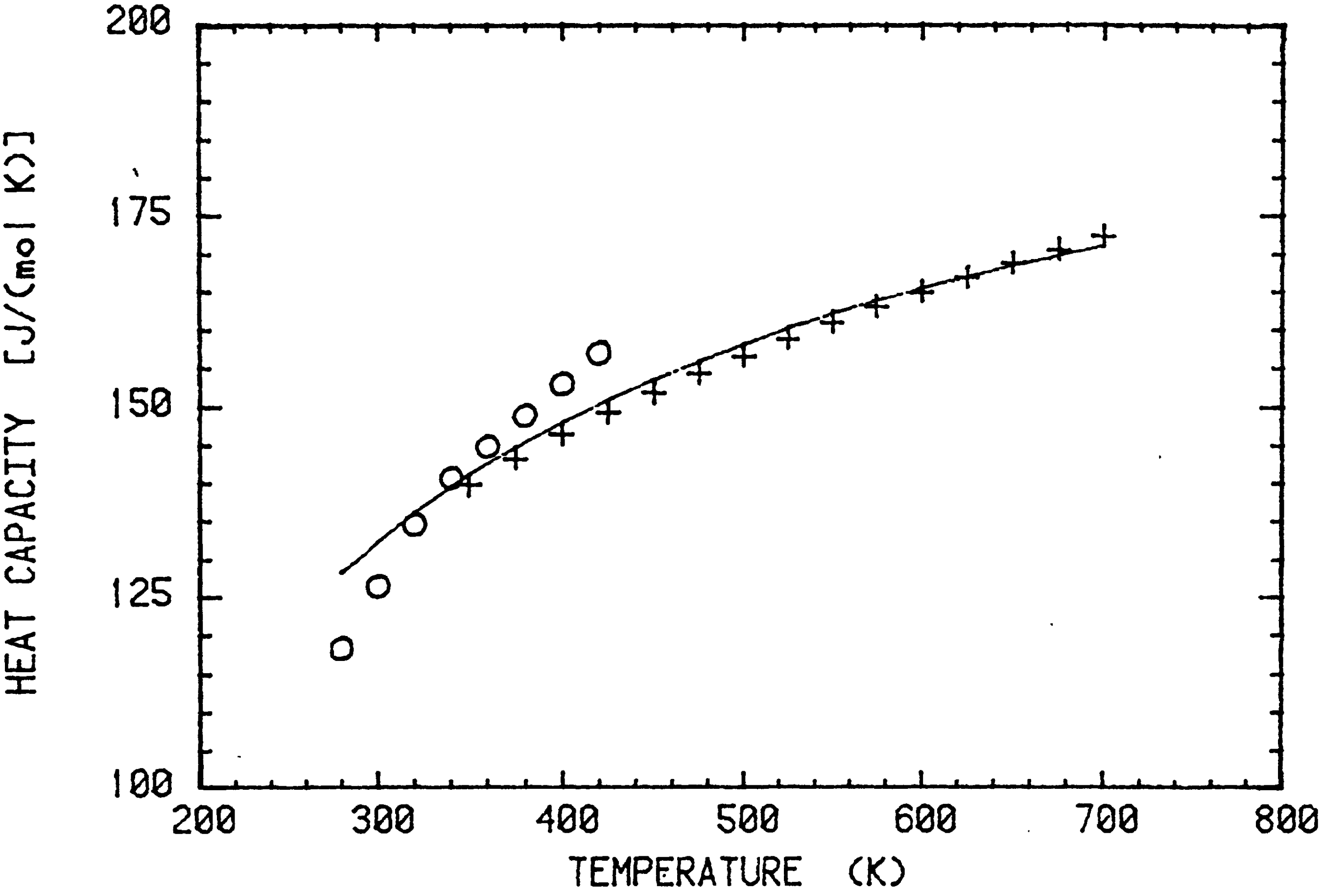

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Figure 7.36

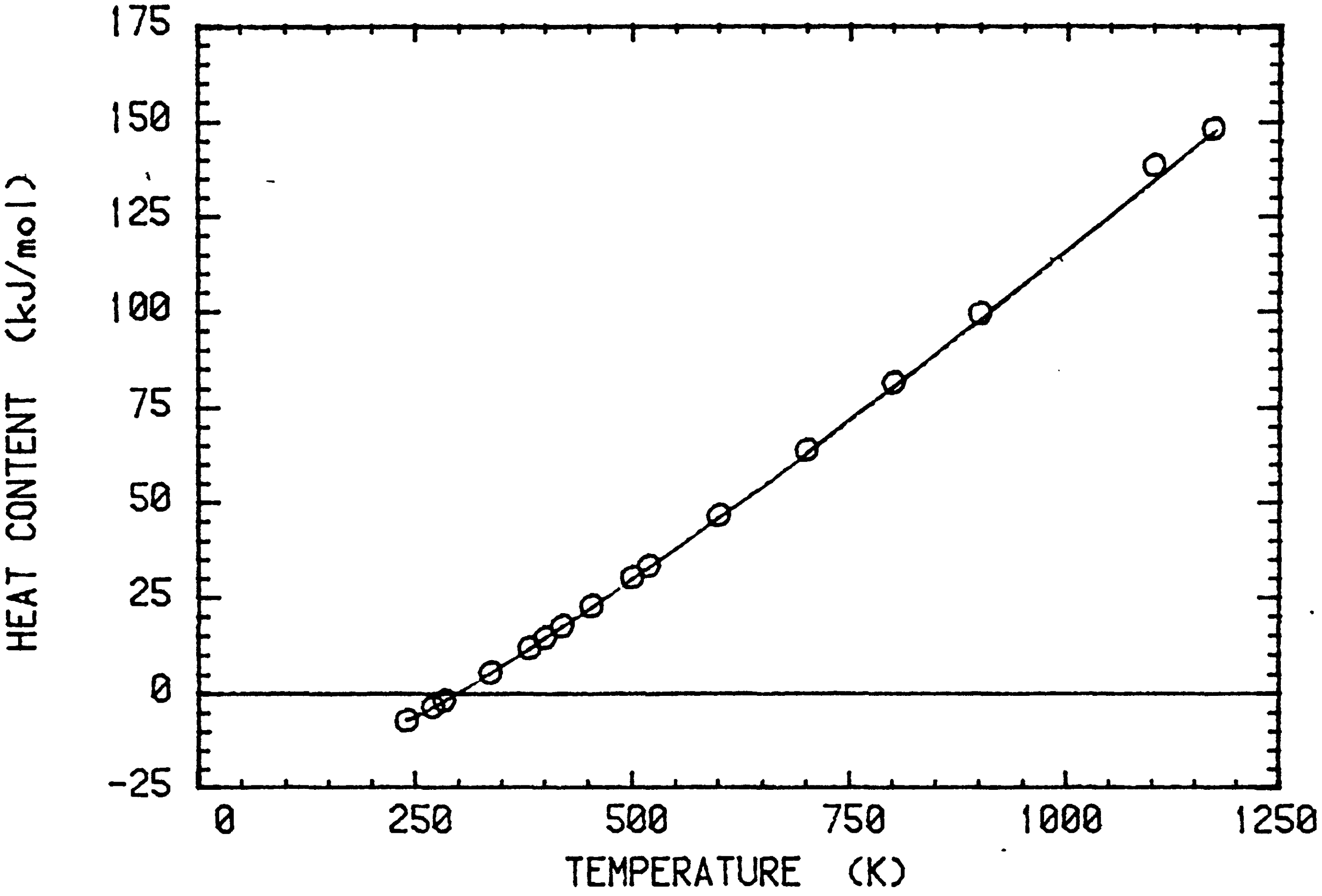


Figure 7.37

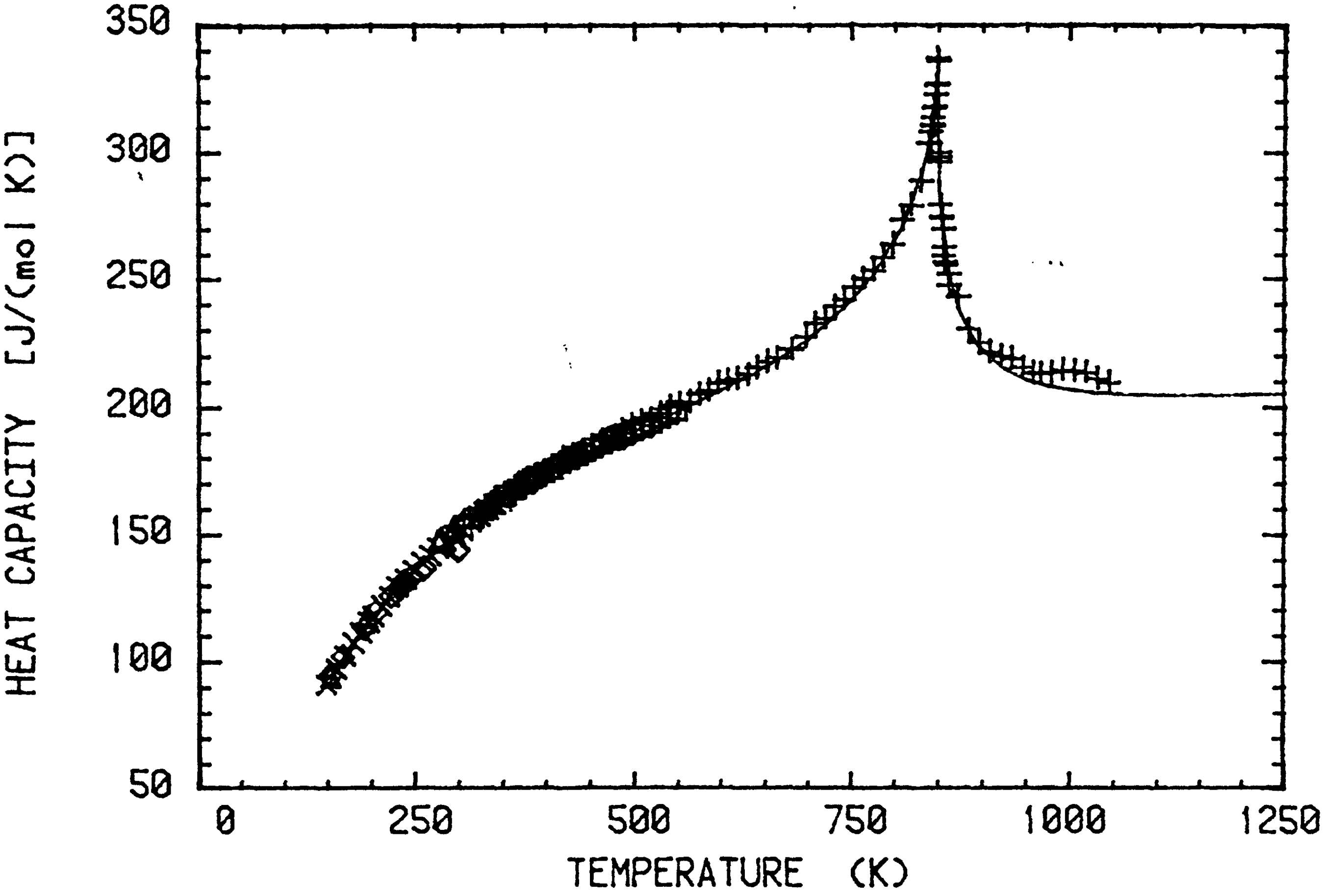
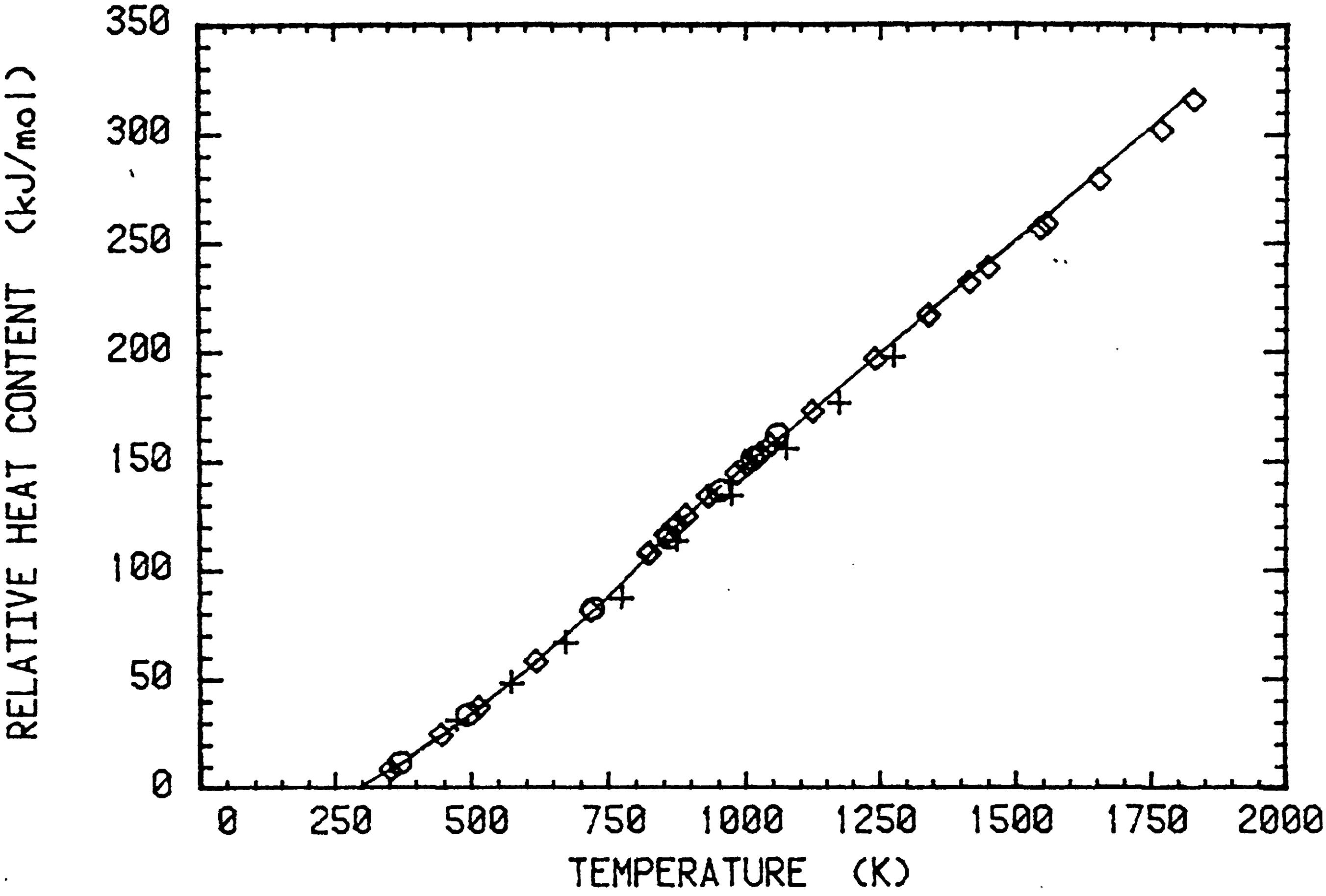
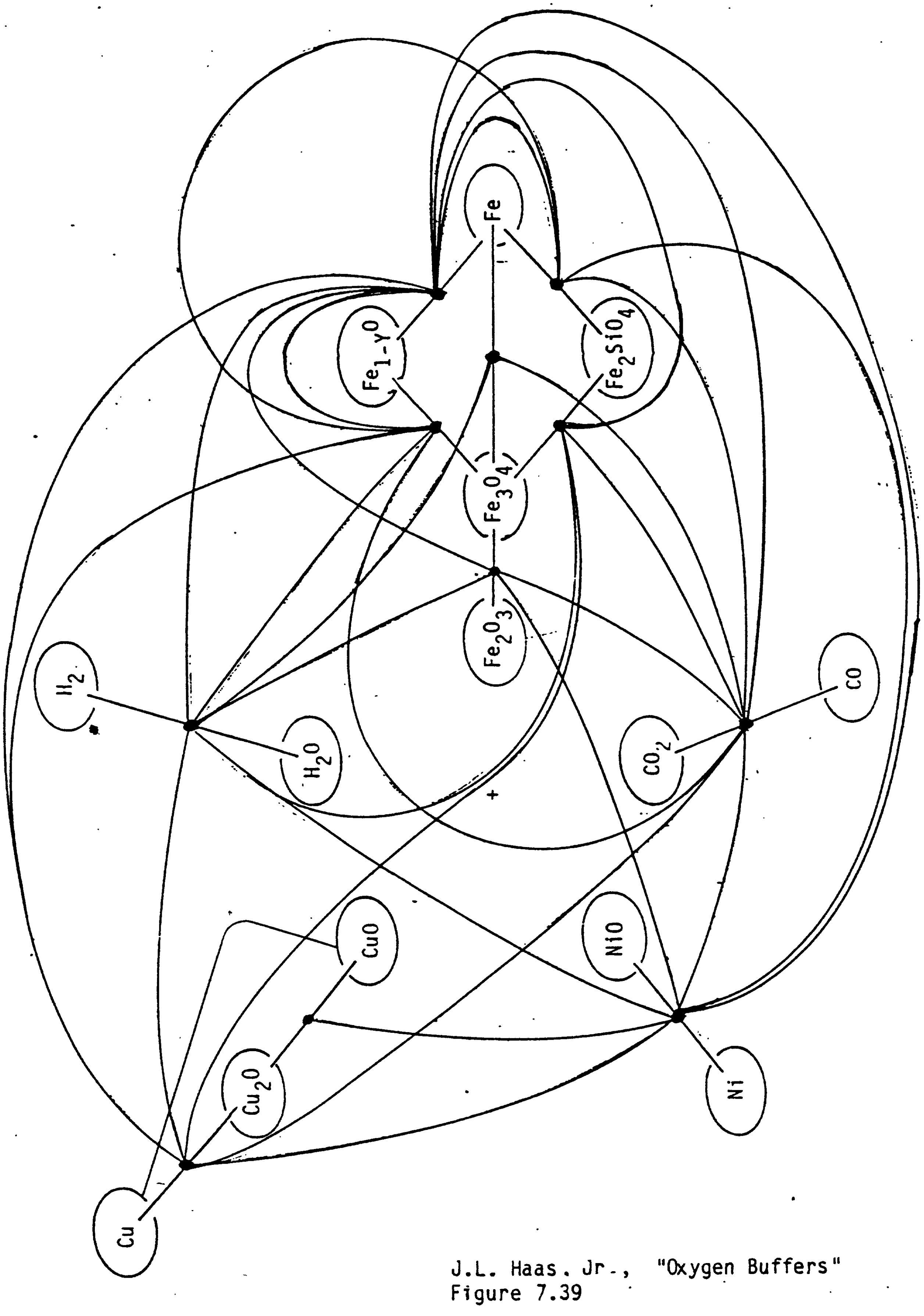

HEAT CAPACITY [J/(mol K)]
350
300
250
200
150
100
50
0
250
500
750
1000
1250
TEMPERATURE (K)

Figure 7.38


RELATIVE HEAT CONTENT (kJ/mol)
350
300
250
200
150
100
50
0
0
250
500
750
1000
1250
1500
1750
2000
TEMPERATURE (K)



J.L. Haas. Jr., "Oxygen Buffers"
Figure 7.39

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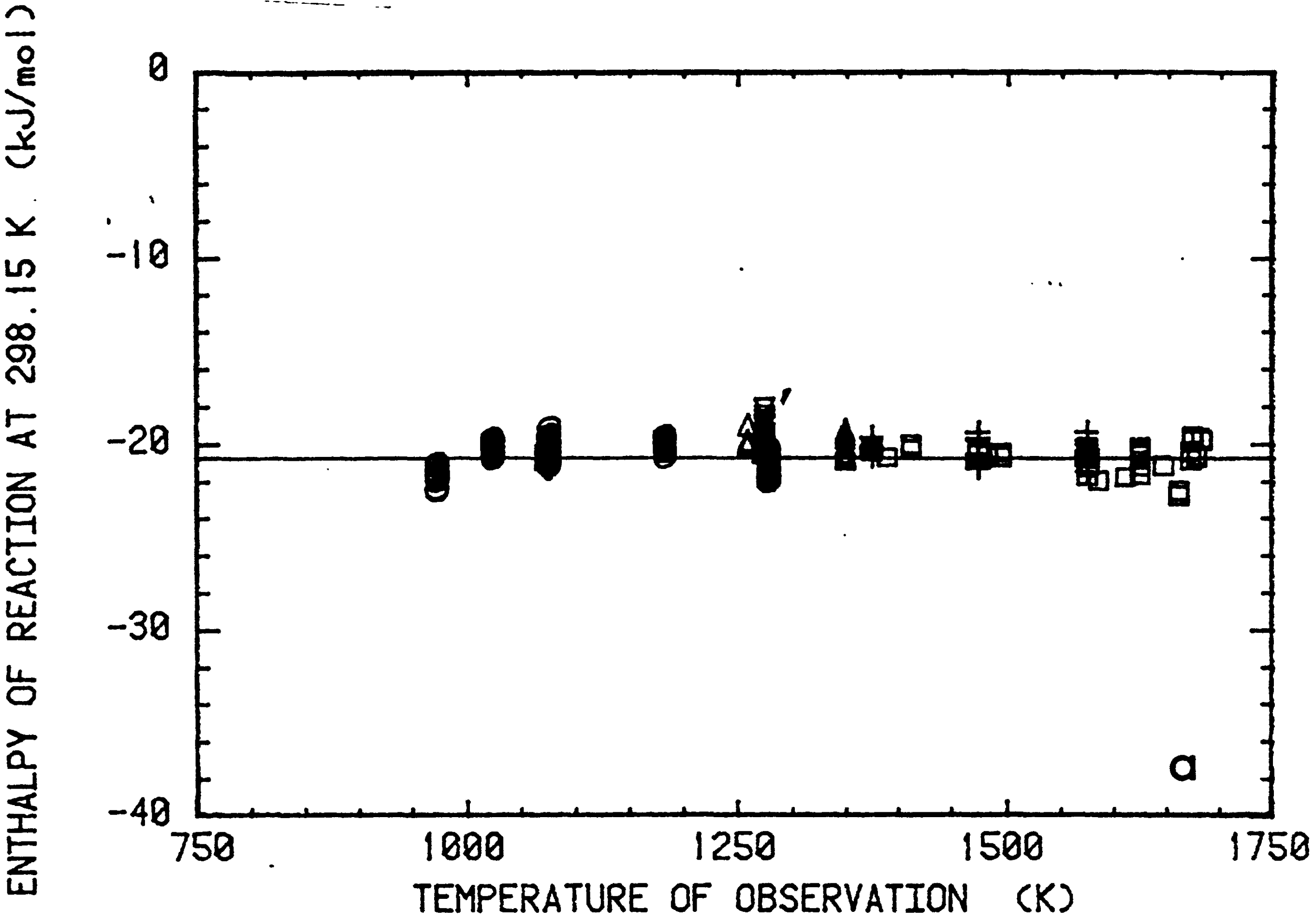
Figure 7.40, b



493

Figure 7.40,

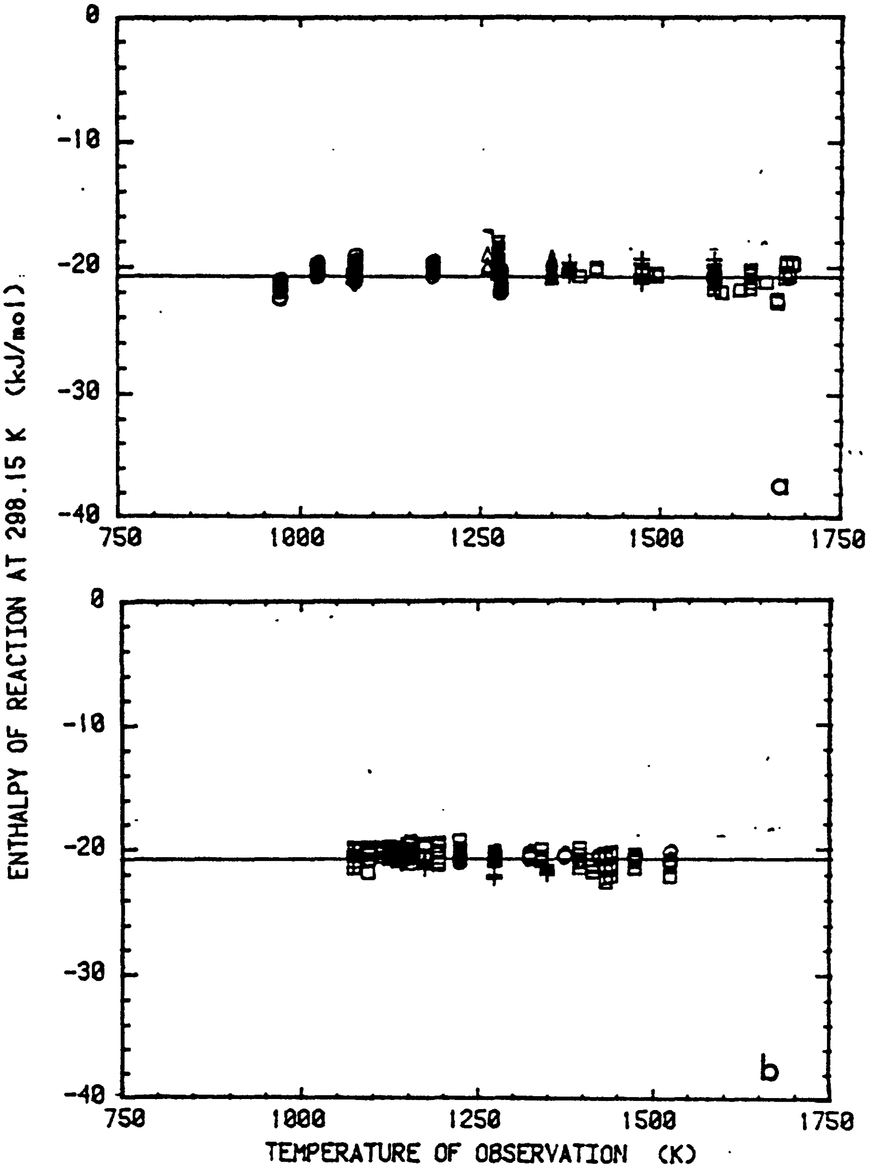

0
-10
-20
-30
-40
750
1000
1250
1500
1750
a
b
ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
TEMPERATURE OF OBSERVATION (K)

Figure 7.41.

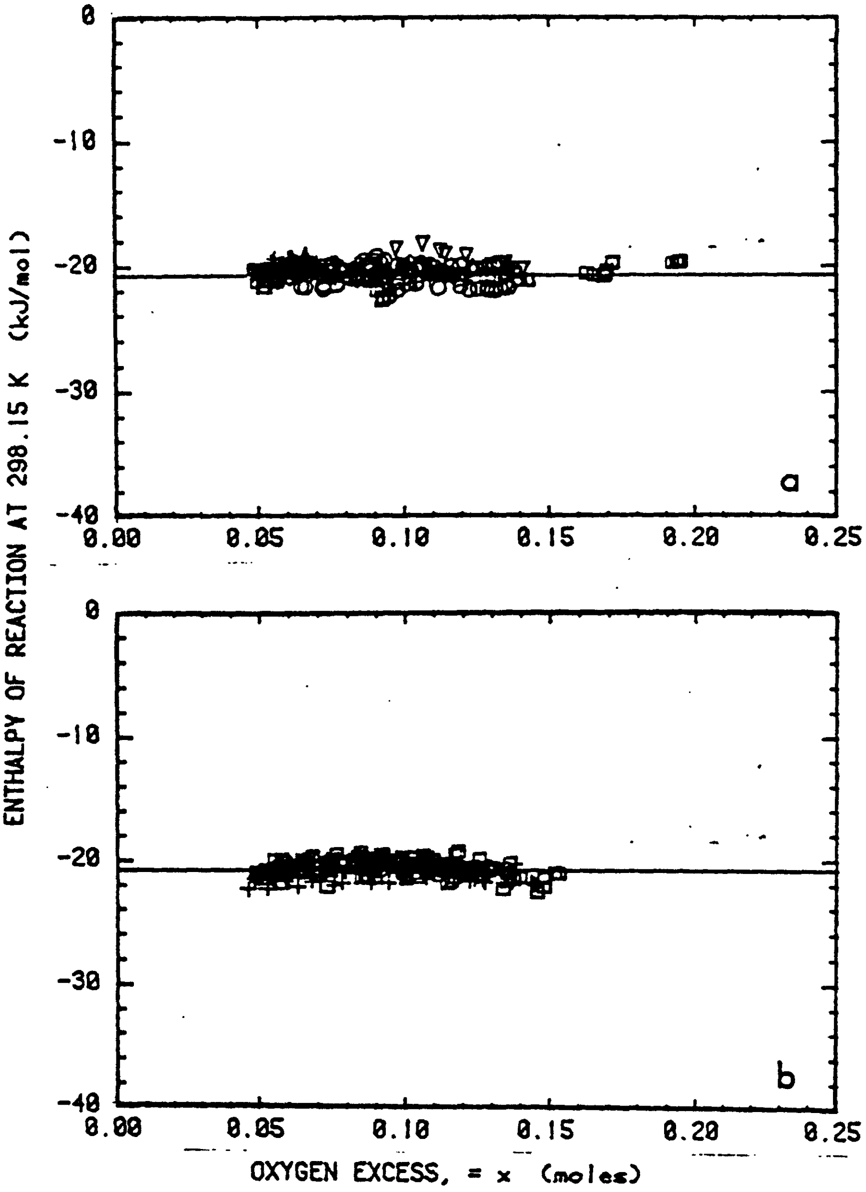

ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
0
-10
-20
-30
-40
a
0.00
0.05
0.10
0.15
0.20
0.25
b
OXYGEN EXCESS, = x (moles)

Figure 7.42

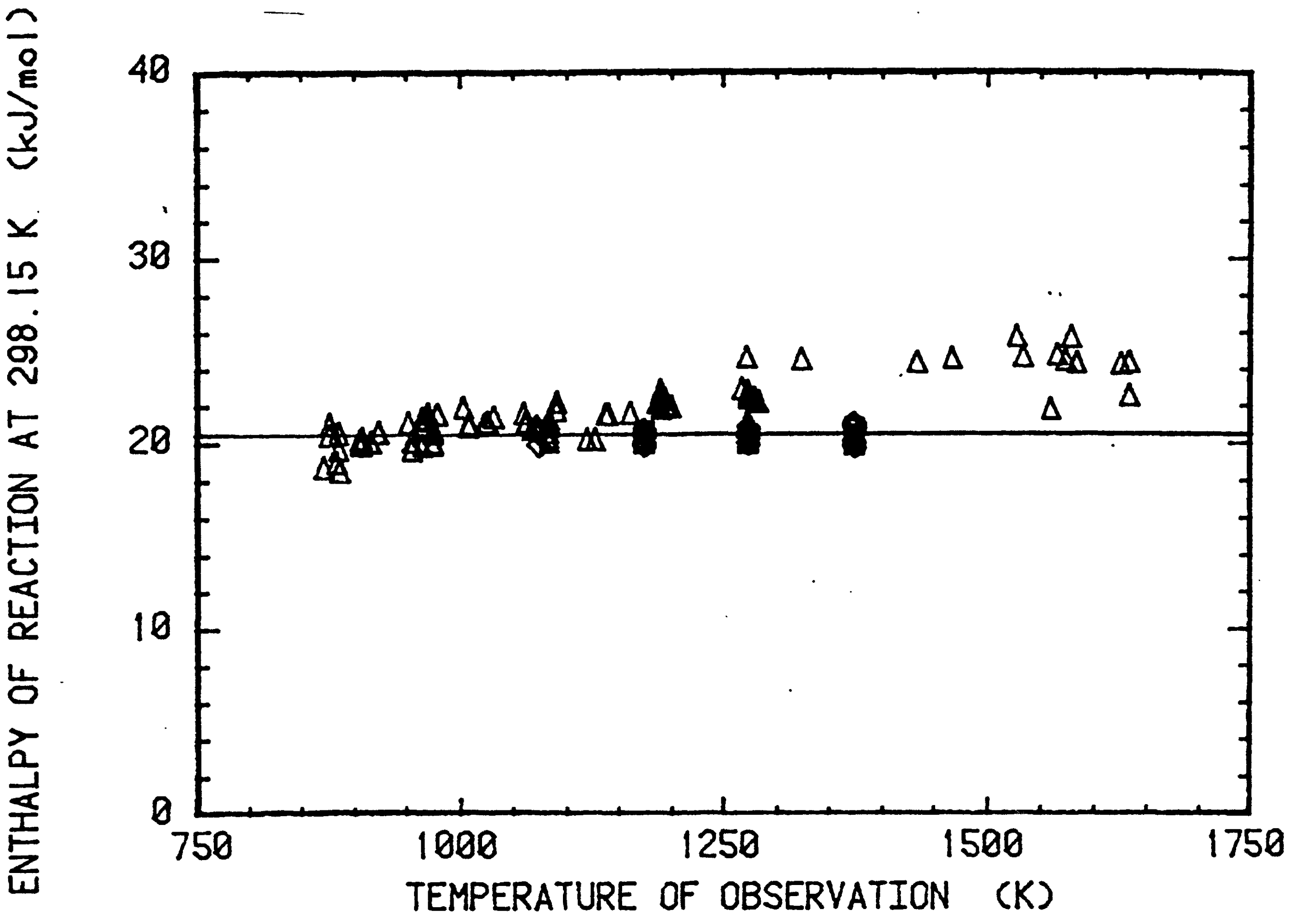

ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
40
30
20
10
0
750
1000
1250
1500
1750
TEMPERATURE OF OBSERVATION (K)

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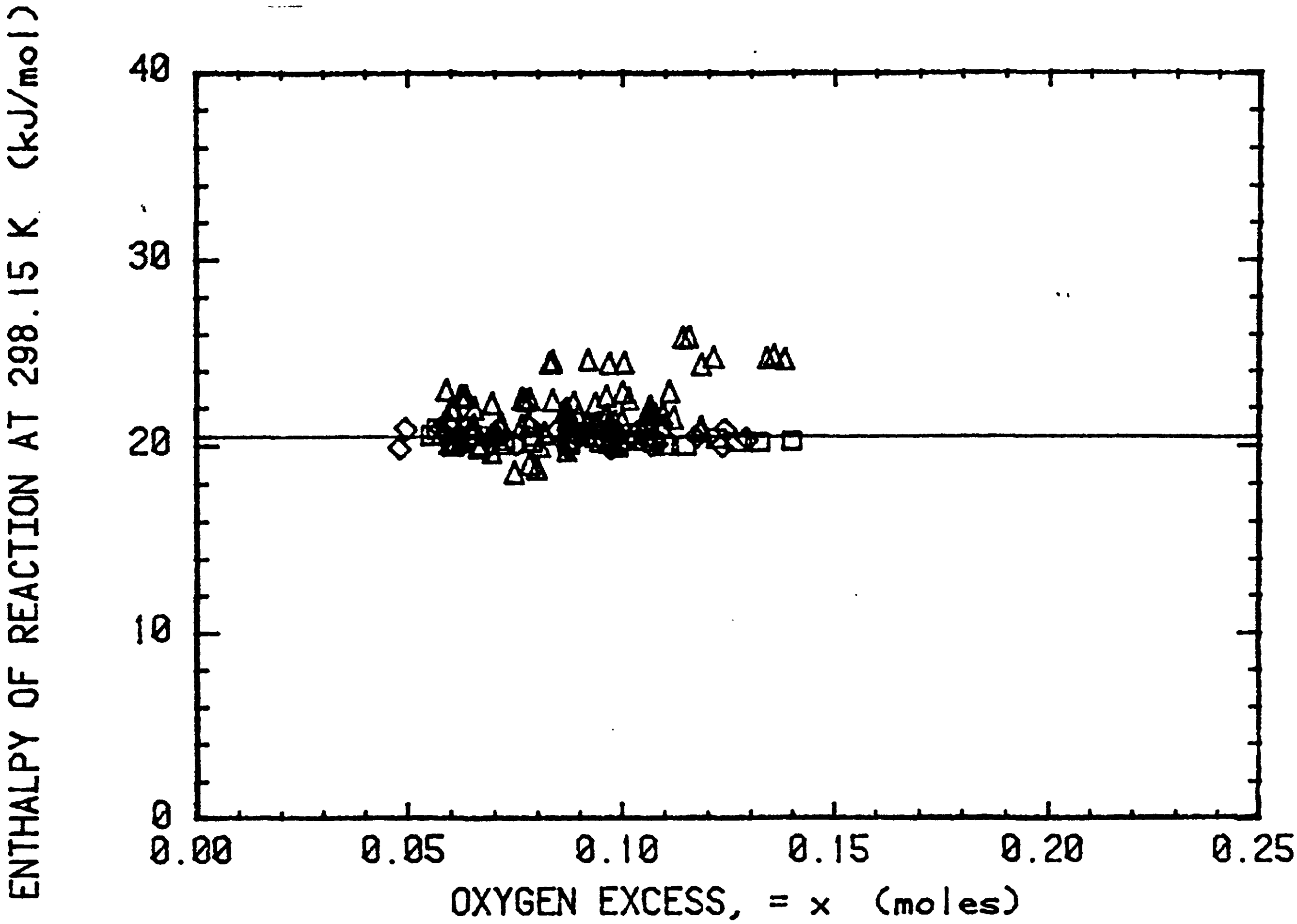
Figure 7.43



497

Figure 7.44

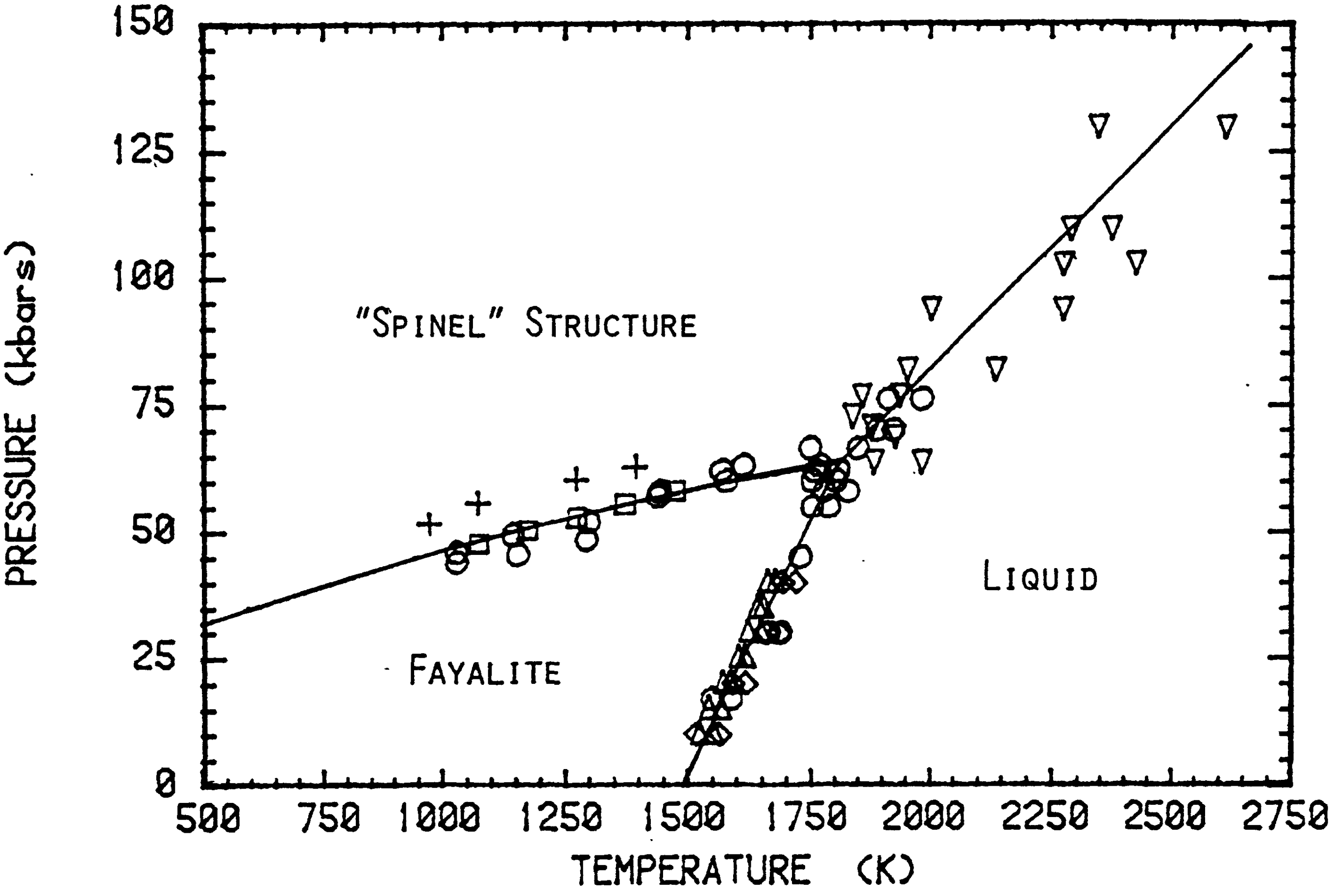

150
125
100
75
50
25
0
PRESSURE (kbars)
500
750
1000
1250
1500
1750
2000
2250
2500
2750
TEMPERATURE (K)
"SPINEL" STRUCTURE
FAYALITE
LIQUID

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Figure 7.45

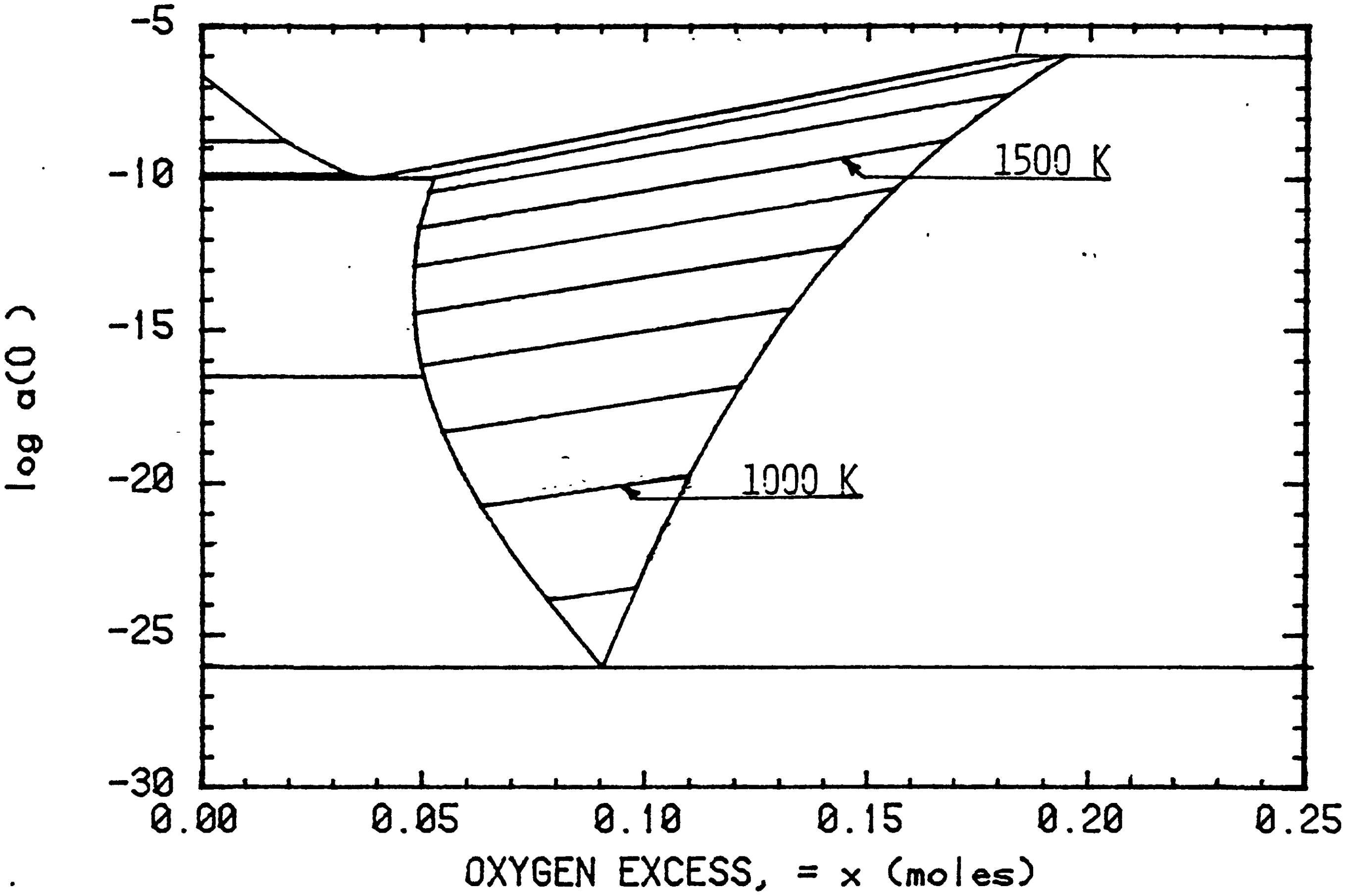

Figure 7.46

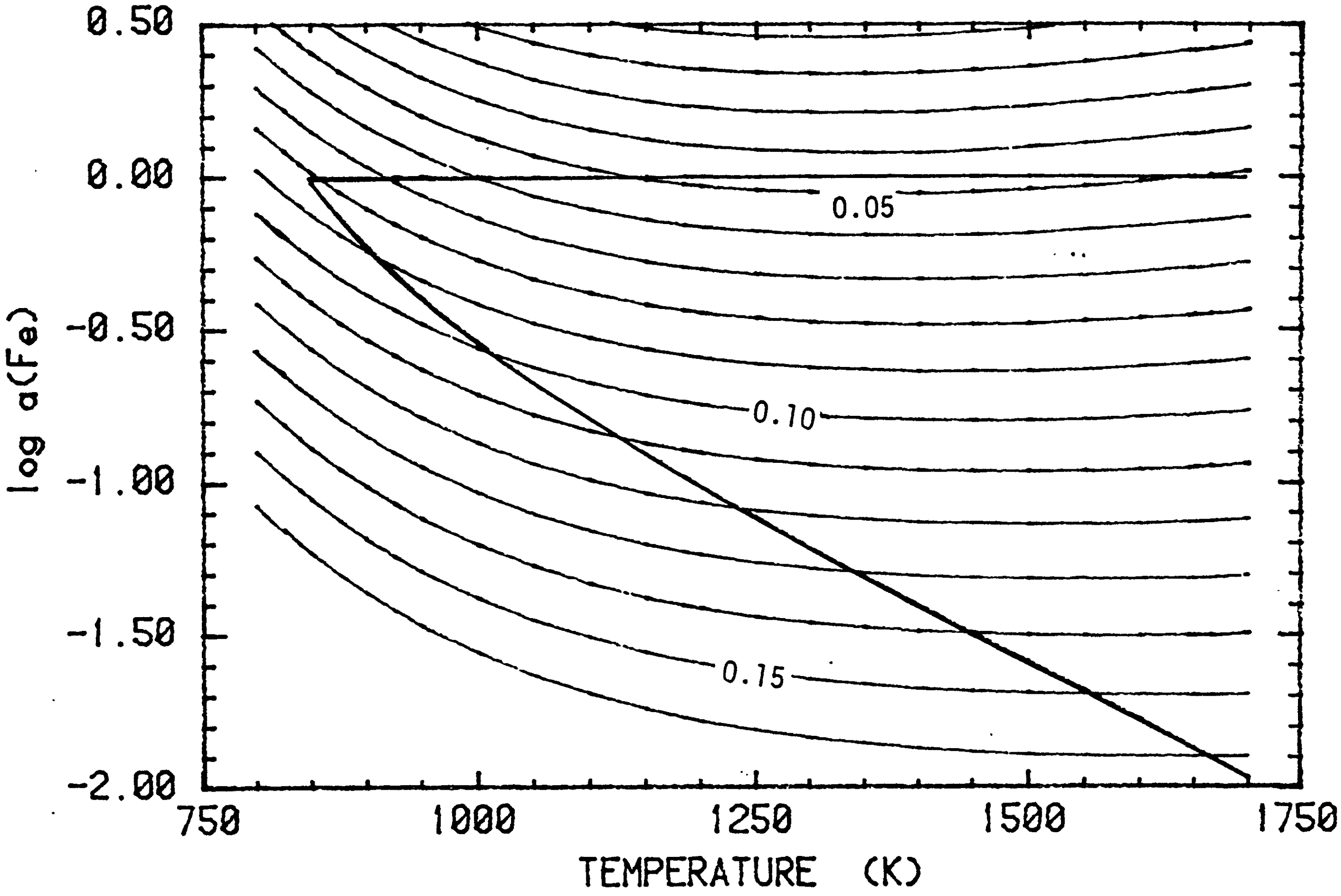
0.50
0.00
-0.50
-1.00
-1.50
-2.00
log a(Fe)
750
1000
1250
1500
1750
TEMPERATURE (K)
0.05
0.10
0.15

Figure 7.47

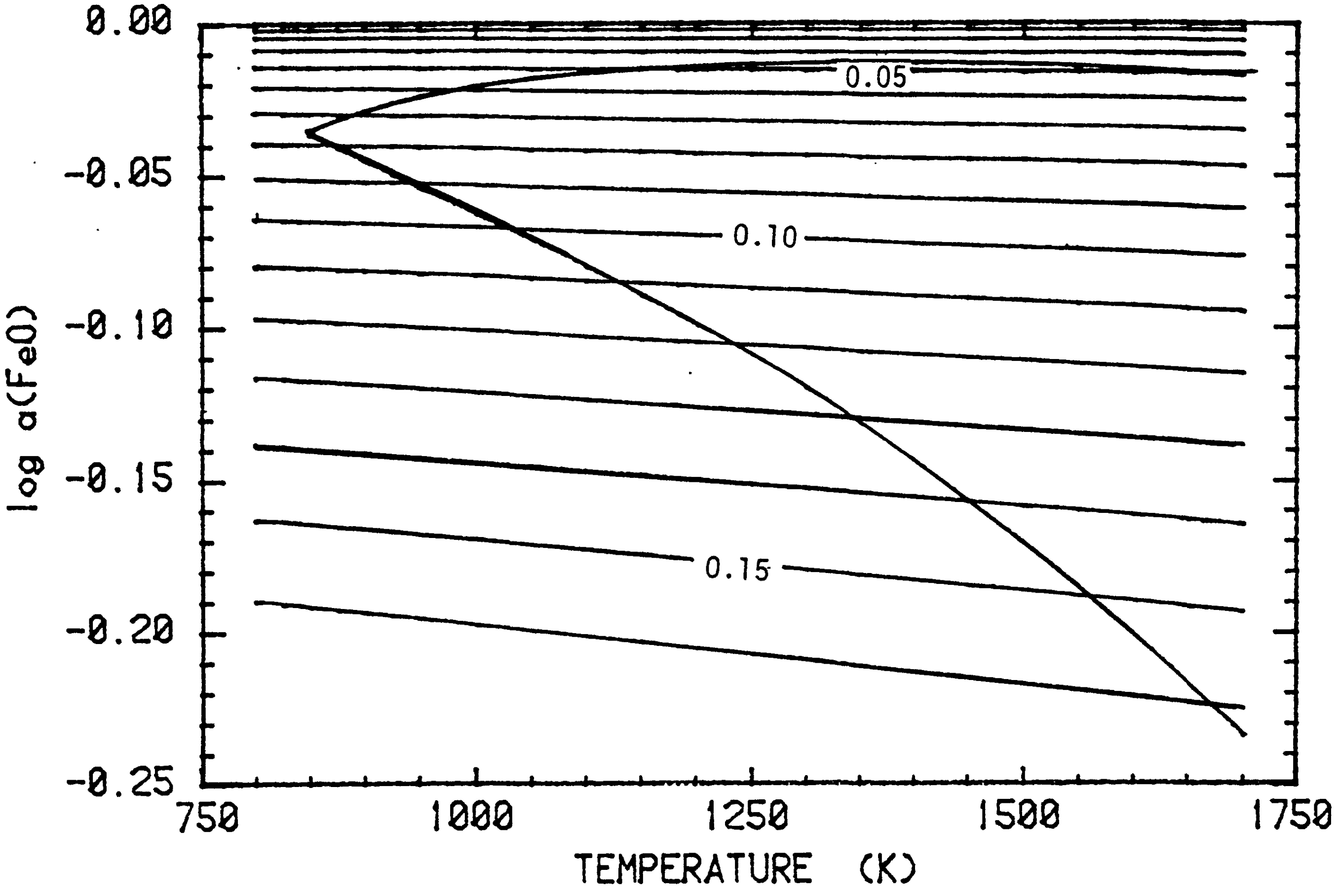
0.00
-0.05
-0.10
-0.15
-0.20
-0.25
log a(FeO)
750
1000
1250
1500
1750
TEMPERATURE (K)
0.05
0.10
0.15

Figure 7.48

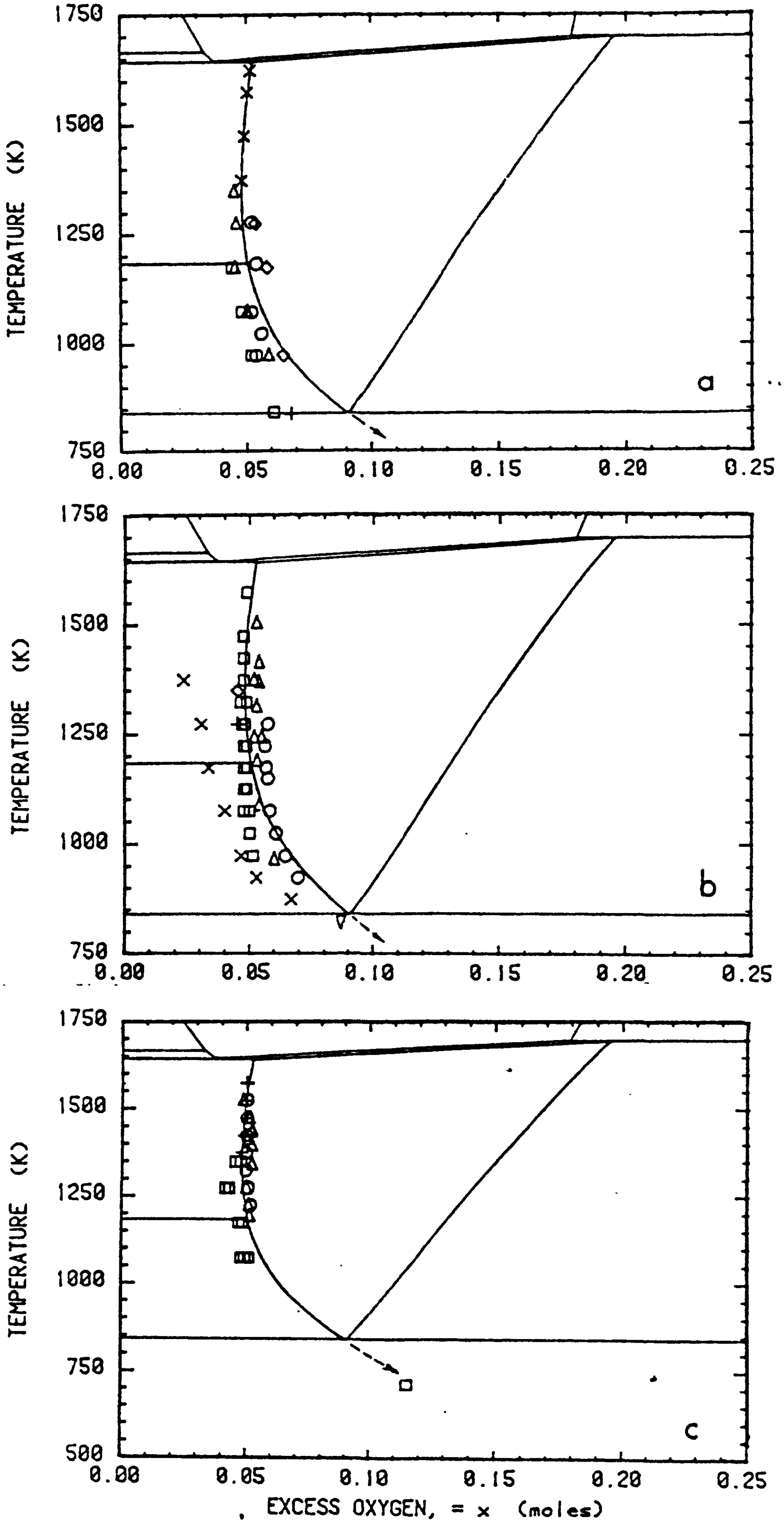
1750
1500
1250
1000
750
500
0.00
0.05
0.10
0.15
0.20
0.25
TEMPERATURE (K)
a
b
c
EXCESS OXYGEN, = x (moles)

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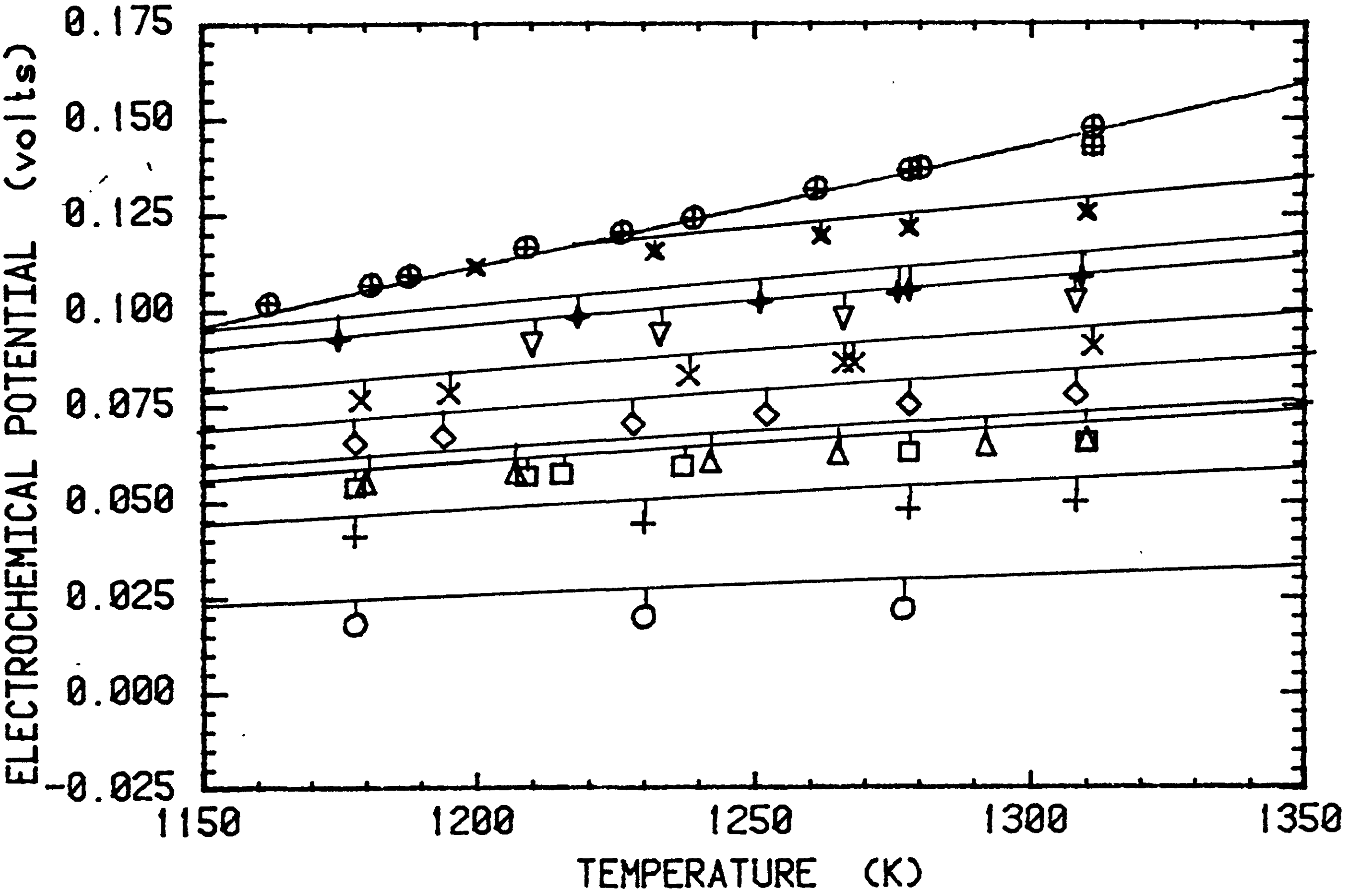
Figure 7.49



503

Figure 7.50

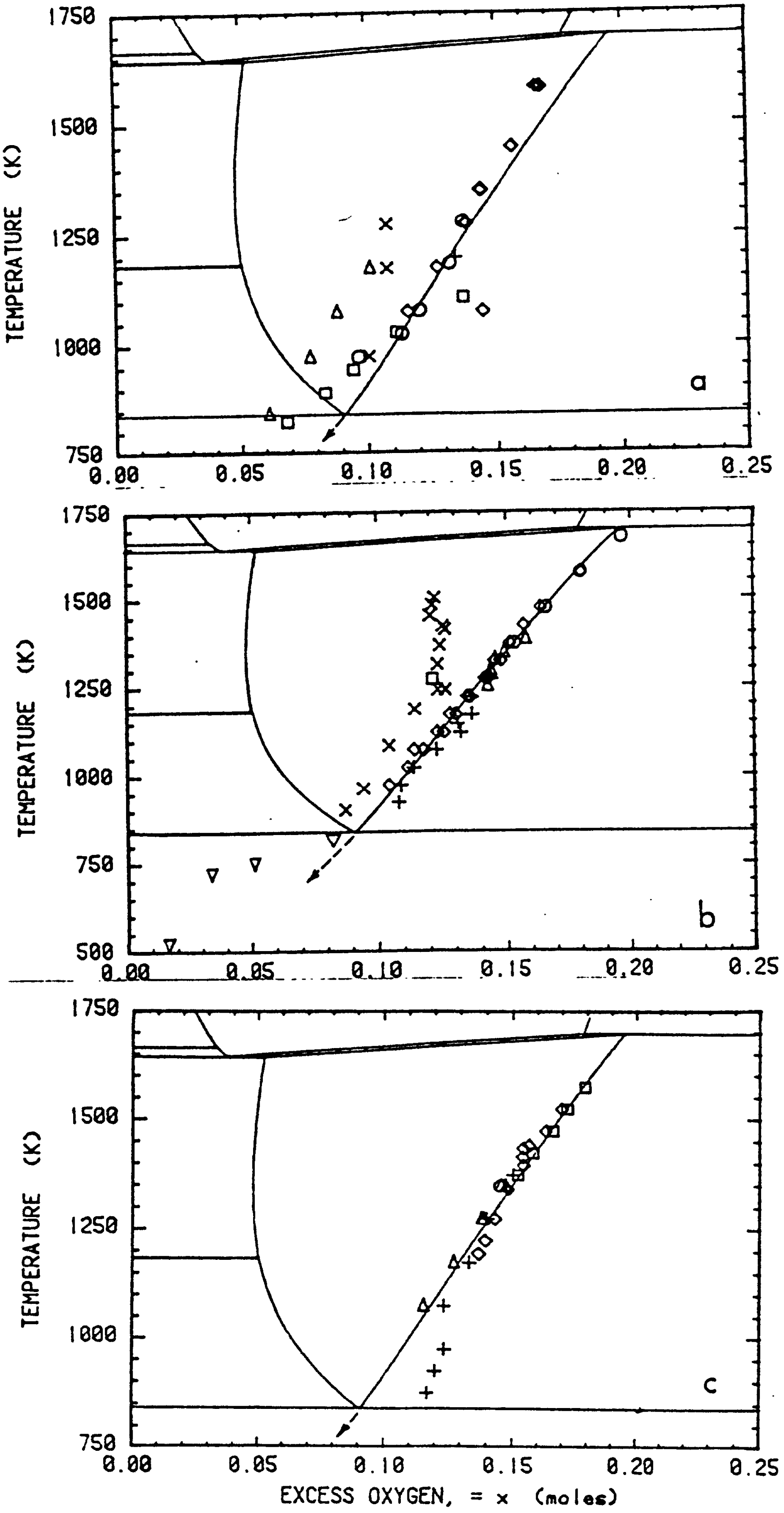

1750
1500
1250
1000
750
500
TEMPERATURE (K)
0.00
0.05
0.10
0.15
0.20
0.25
a
b
c
EXCESS OXYGEN, = x (moles)

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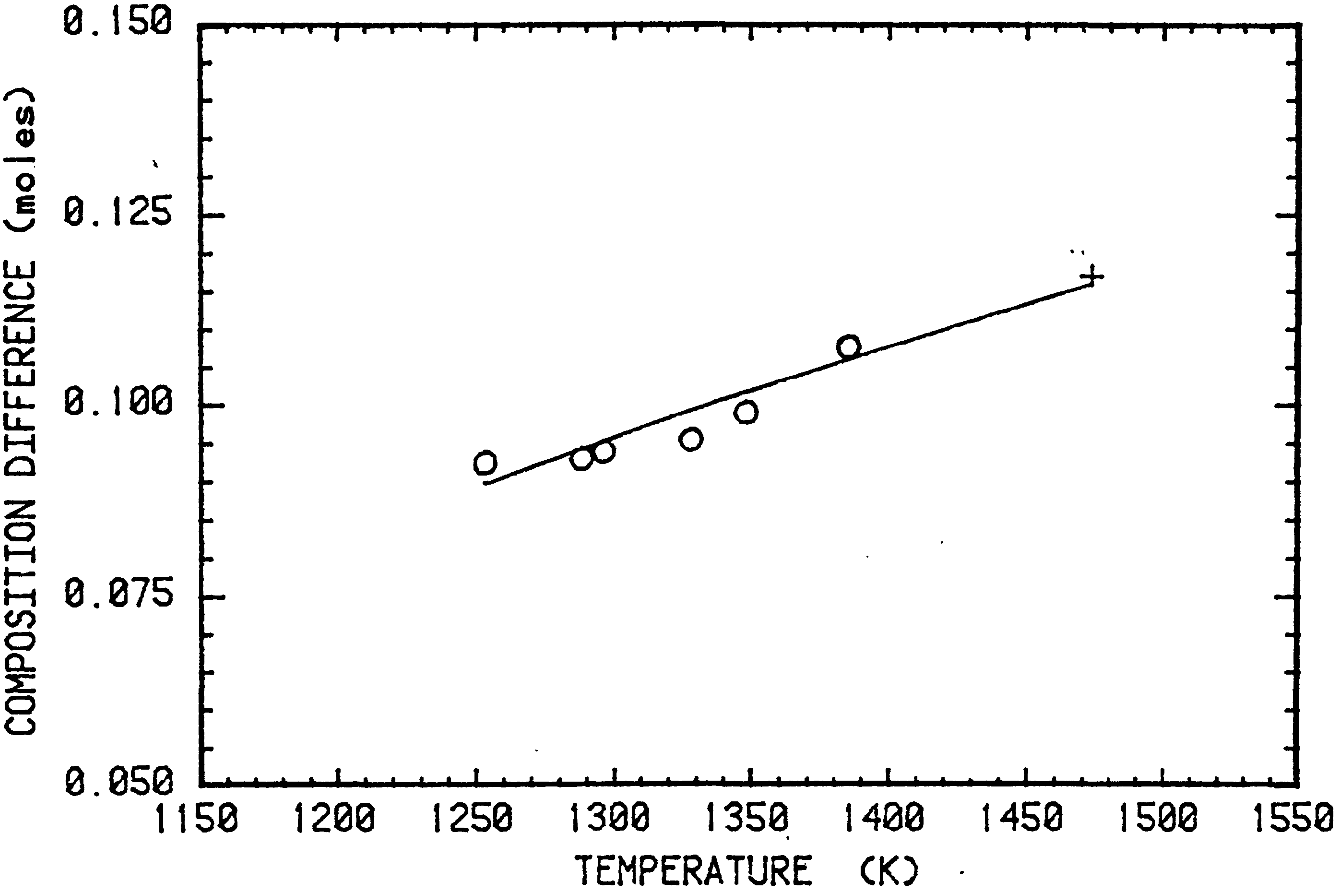
Figure 7.51



505

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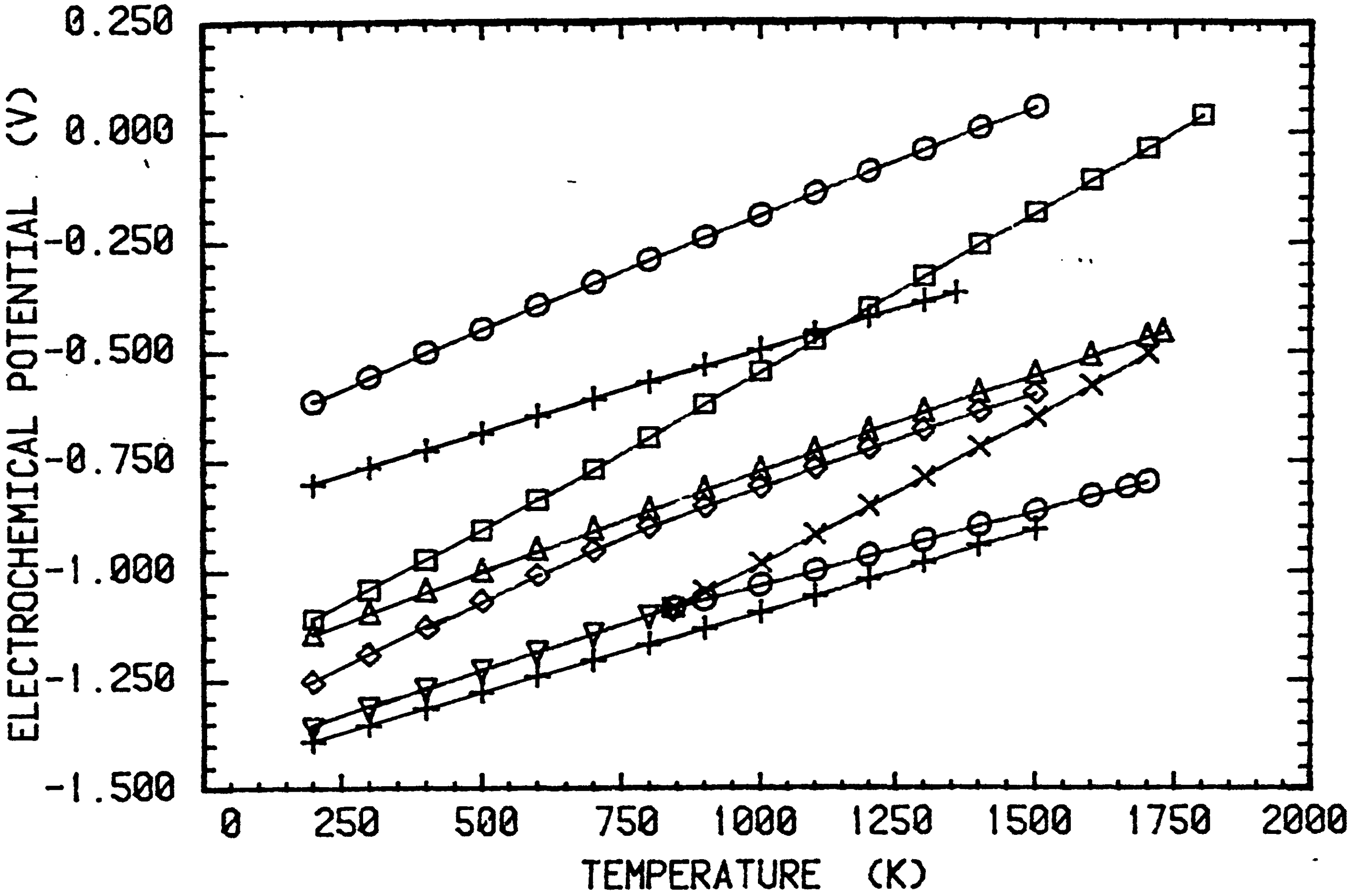
Figure 10.1



506

Figure A.81,

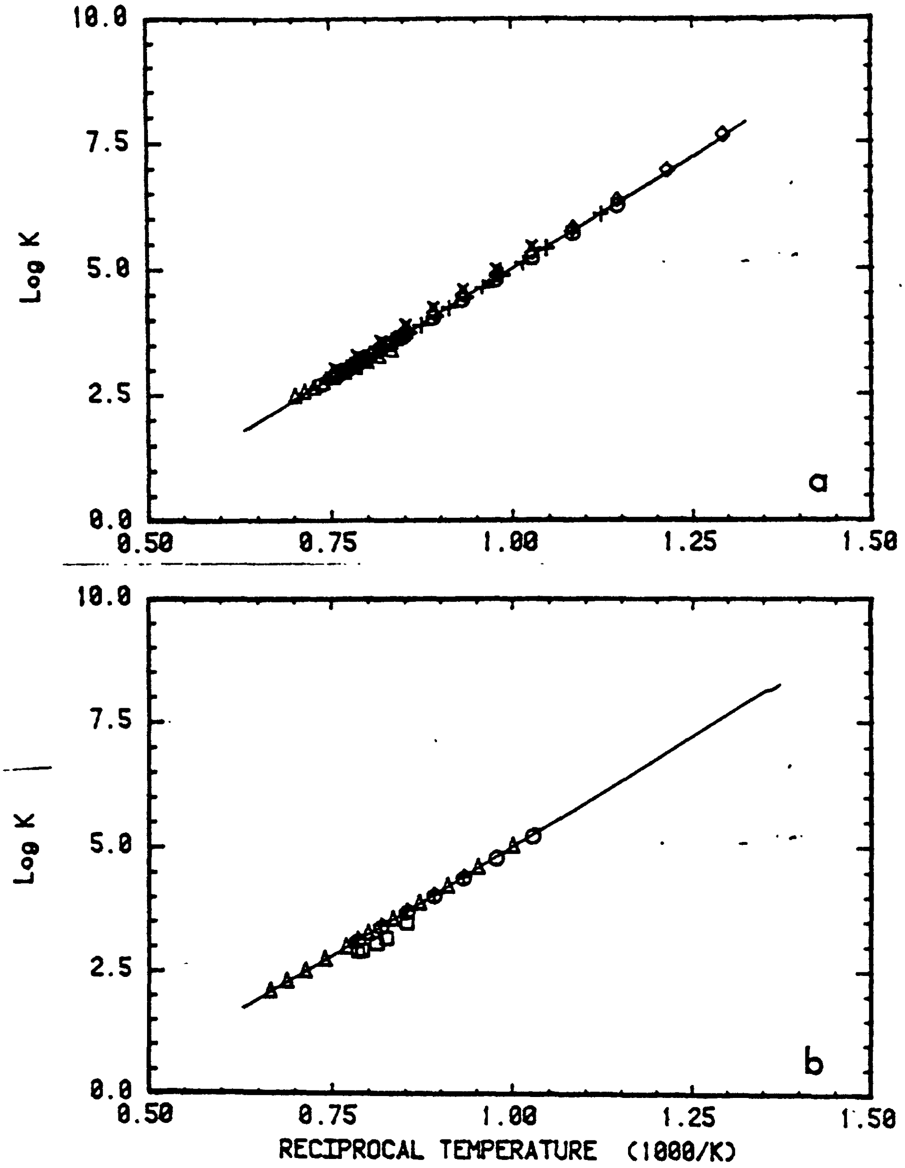
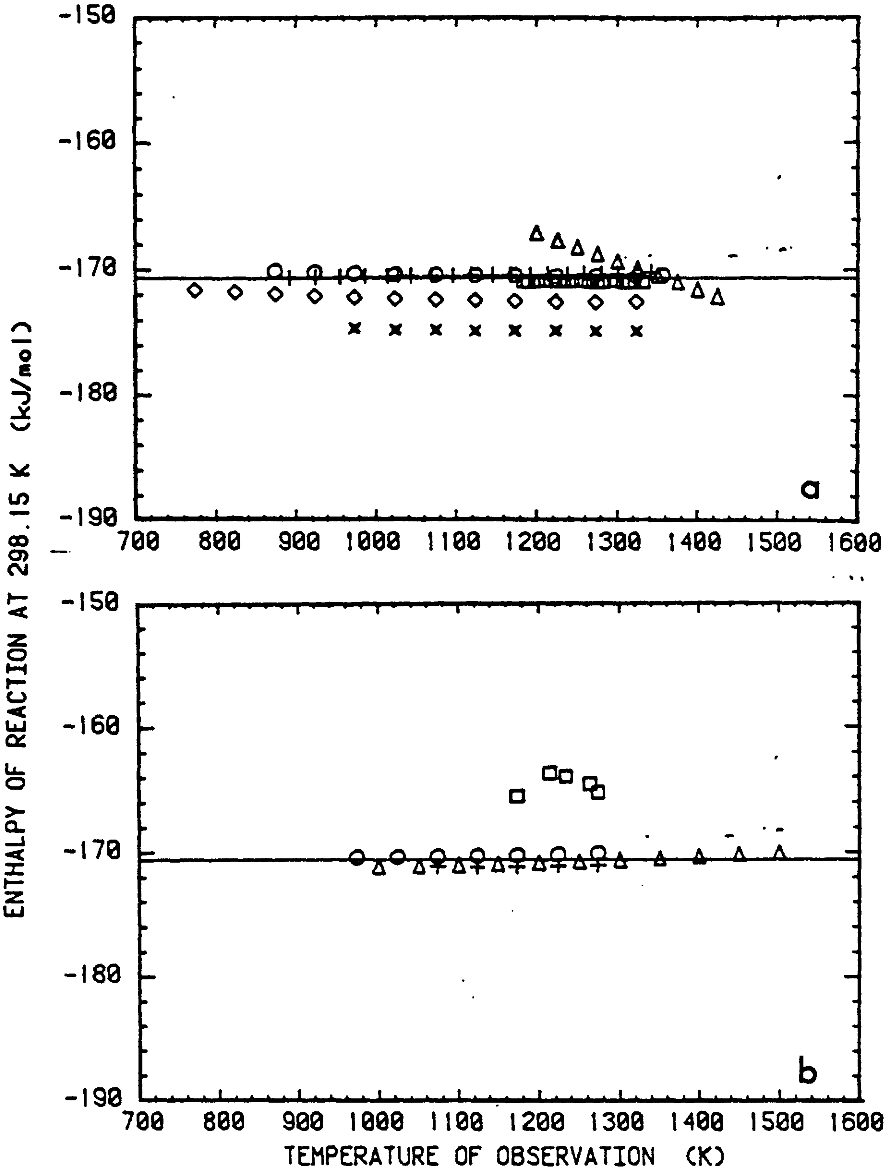
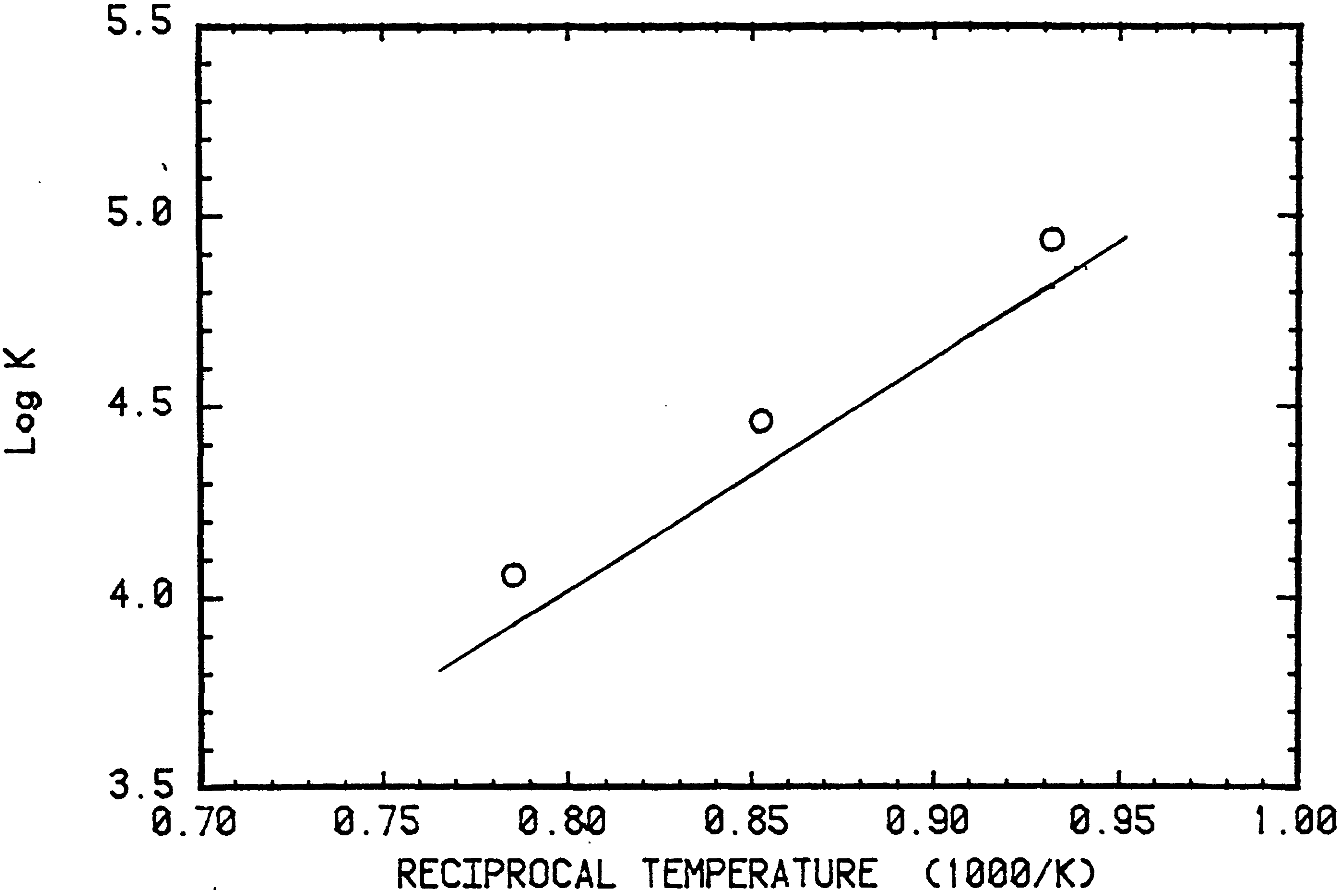

10.0
7.5
5.0
2.5
0.0
Log K
a
0.50
0.75
1.00
1.25
1.50
10.0
7.5
5.0
2.5
0.0
Log K
b
0.50
0.75
1.00
1.25
1.50
RECIPROCAL TEMPERATURE (1000/K)

Figure A.82.



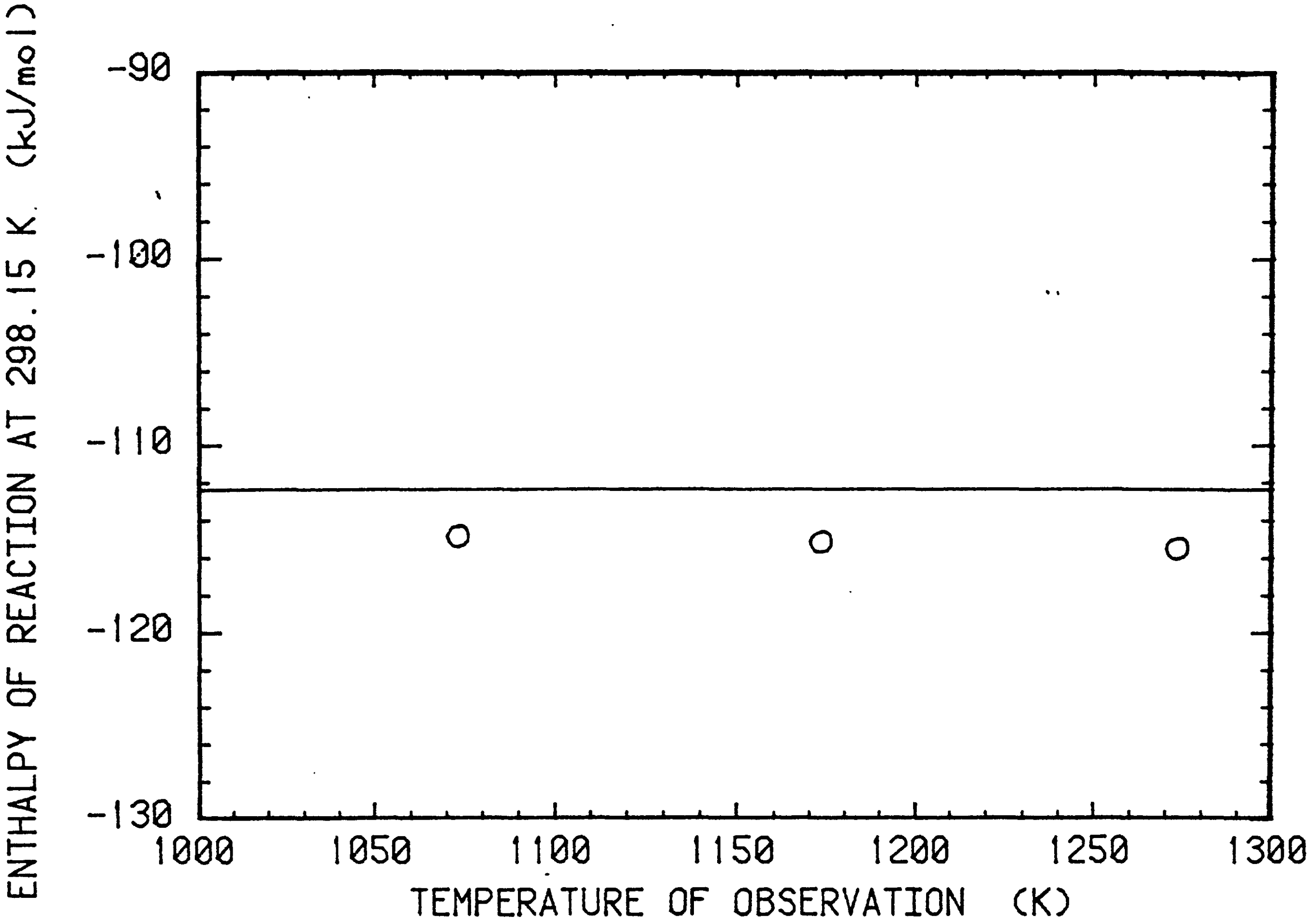
508

Figure A.03



509

Figure A.04



ENTHALPY OF REACTION AT 298.15 K. (kJ/mol)
-90
-100
-110
-120
-130
1000
1050
1100
1150
1200
1250
1300
TEMPERATURE OF OBSERVATION (K)

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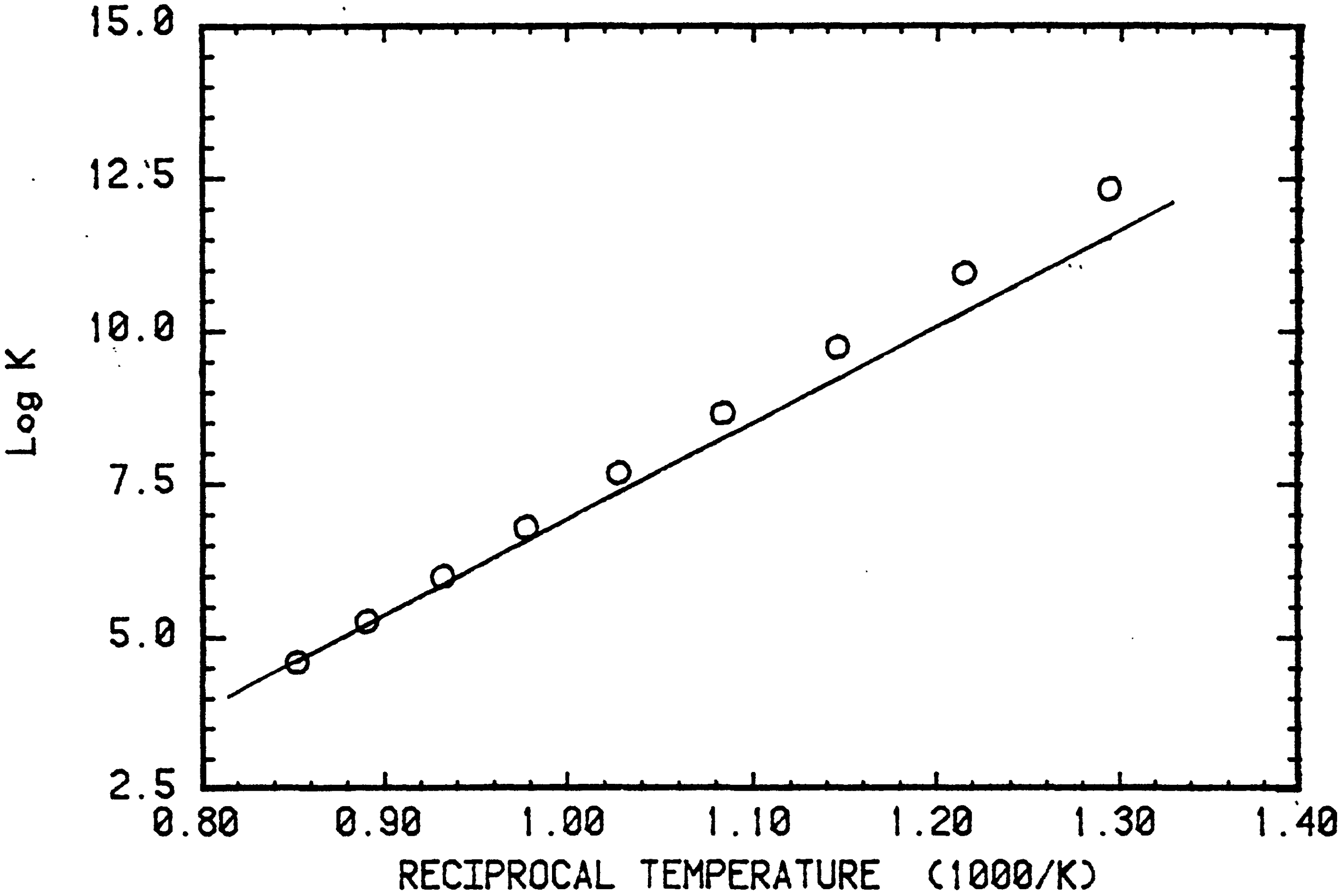
Figure A.05



511

Figure A.06

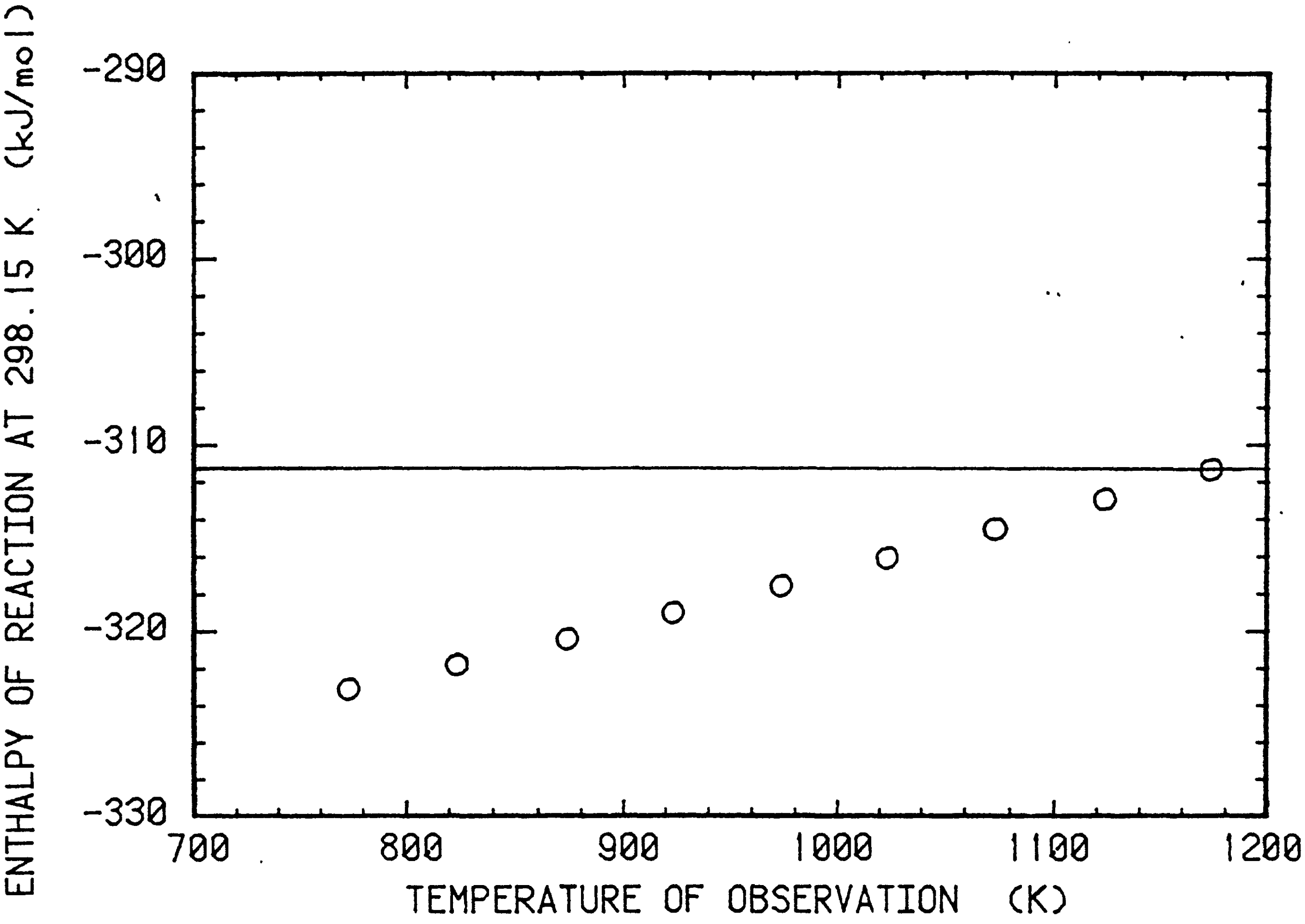

ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
-290
-300
-310
-320
-330
700
800
900
1000
1100
1200
TEMPERATURE OF OBSERVATION (K)

Figure A.87.

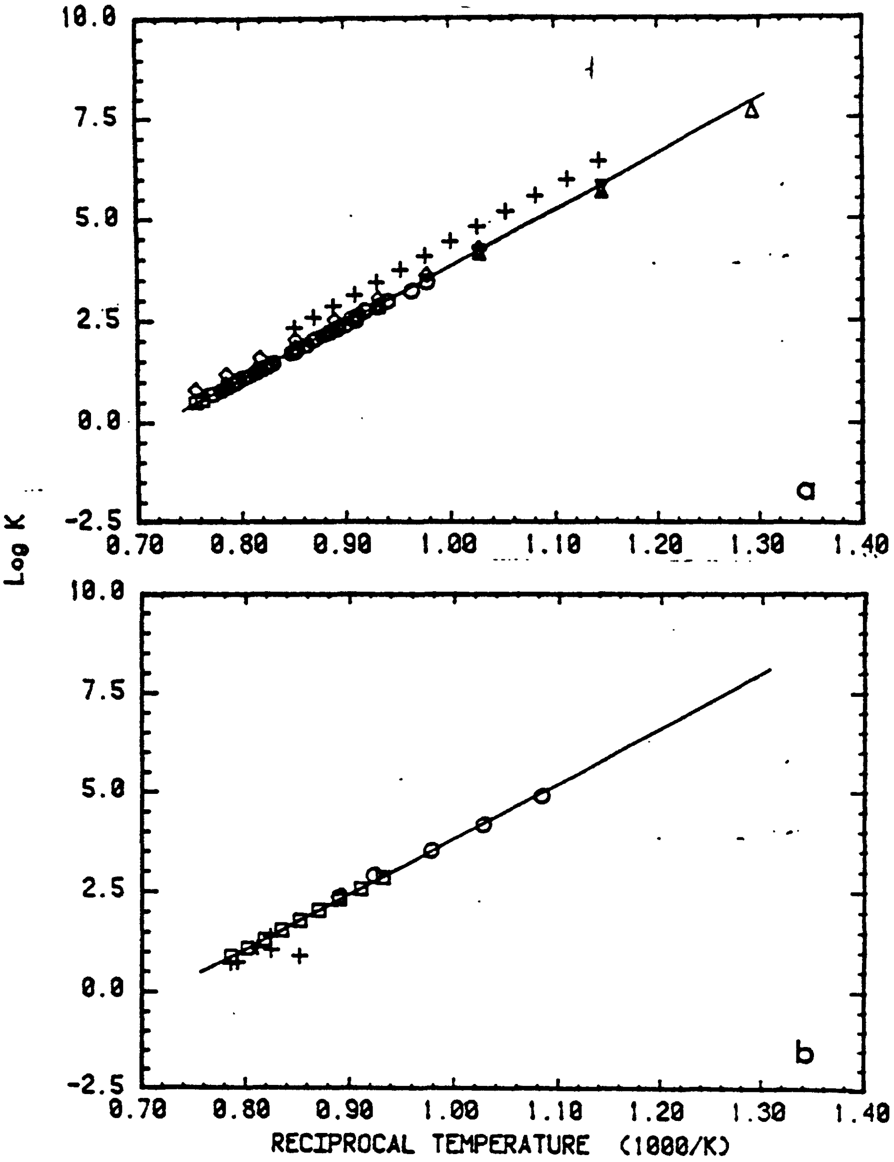
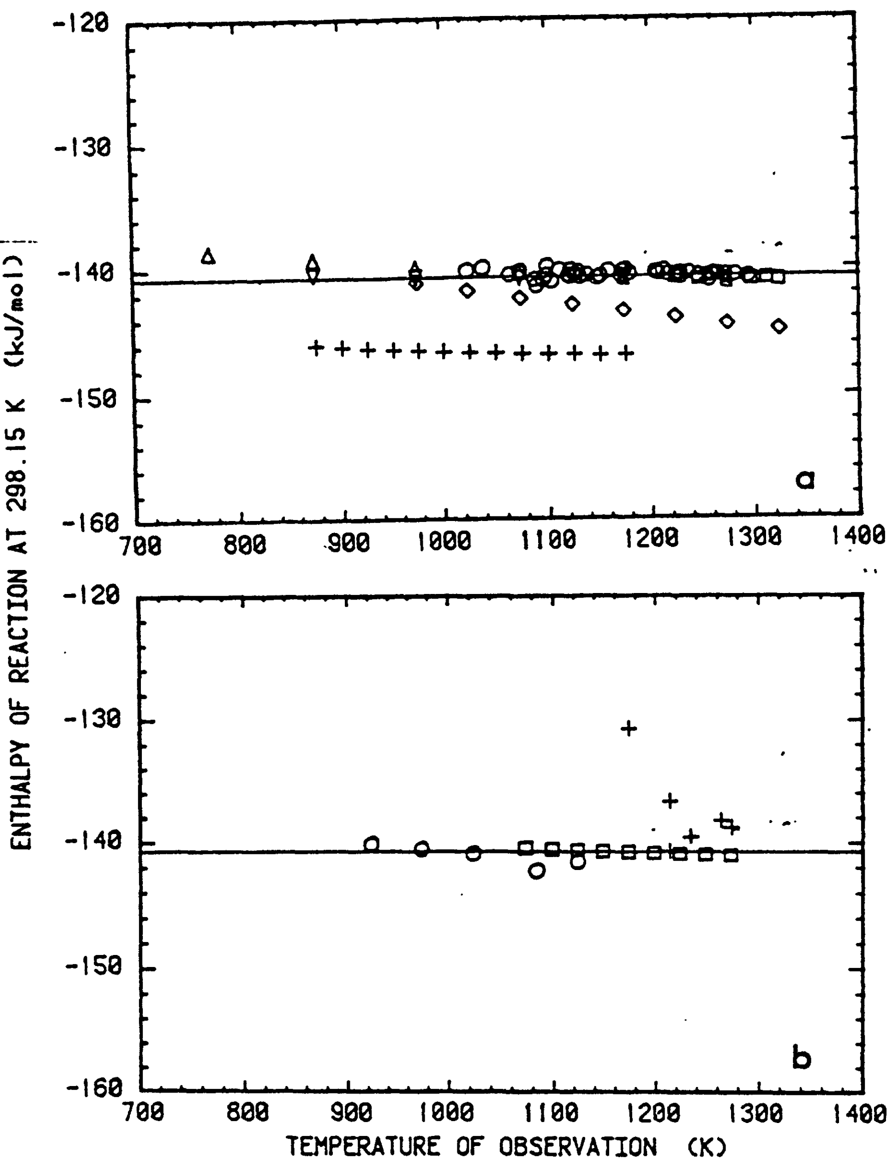

10.0
7.5
5.0
2.5
0.0
-2.5
0.70
0.80
0.90
1.00
1.10
1.20
1.30
1.40
a
Log K
b
RECIPROCAL TEMPERATURE (1000/K)

Figure A.06.



514

Figure A.88.

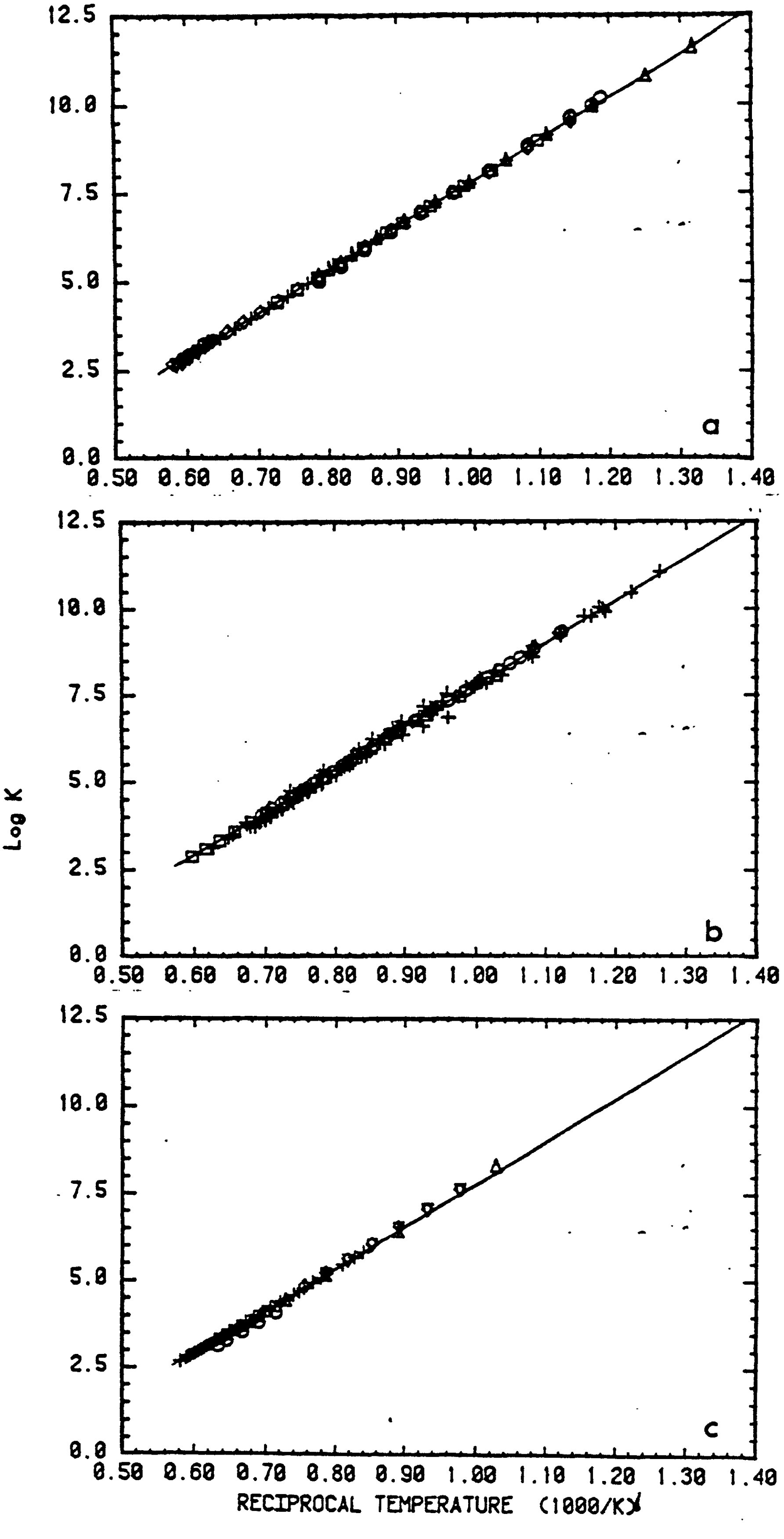
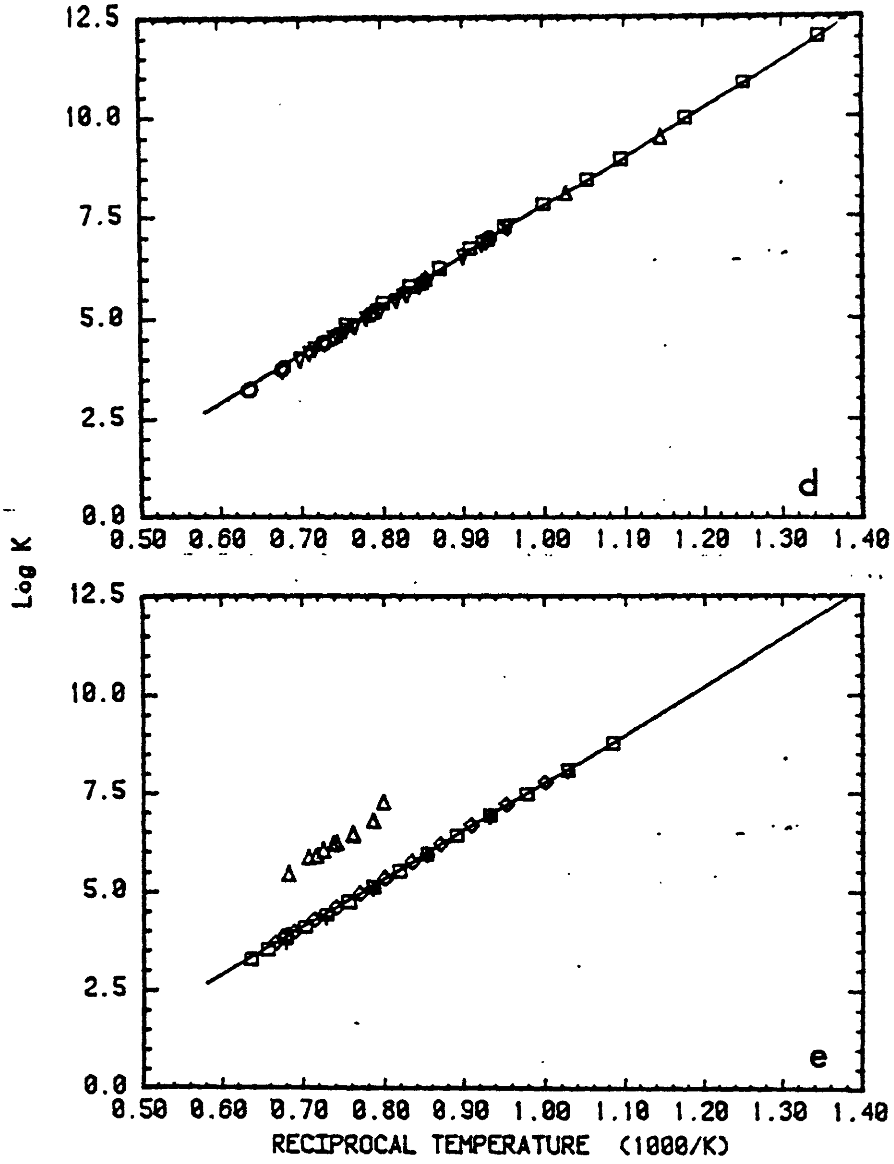
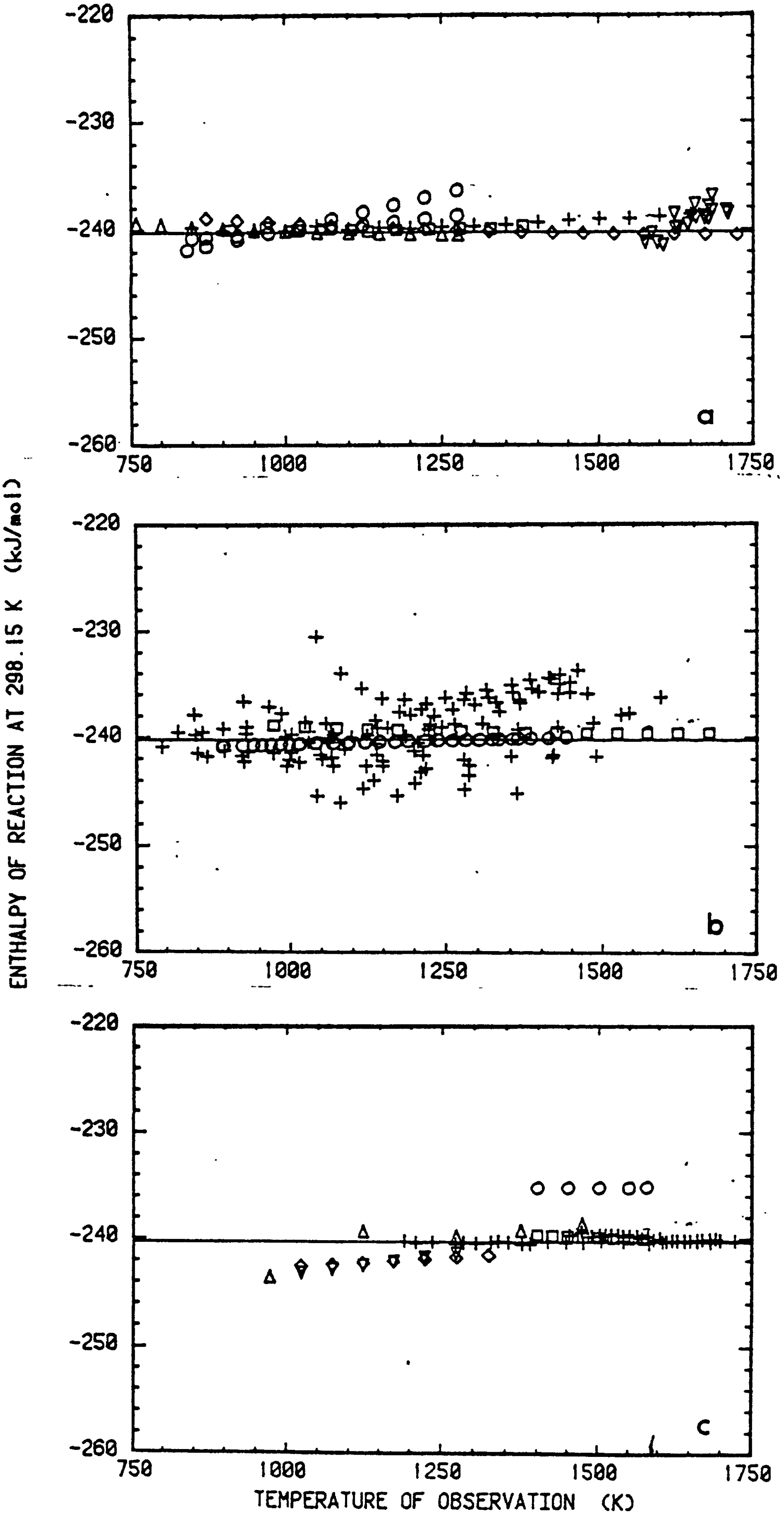

12.5
10.0
7.5
5.0
2.5
0.0
a
0.50 0.60 0.70 0.80 0.90 1.00 1.10 1.20 1.30 1.40
12.5
10.0
7.5
5.0
2.5
0.0
b
0.50 0.60 0.70 0.80 0.90 1.00 1.10 1.20 1.30 1.40
Log K
12.5
10.0
7.5
5.0
2.5
0.0
c
0.50 0.60 0.70 0.80 0.90 1.00 1.10 1.20 1.30 1.40
RECIPROCAL TEMPERATURE (1000/K)

Figure A.88,



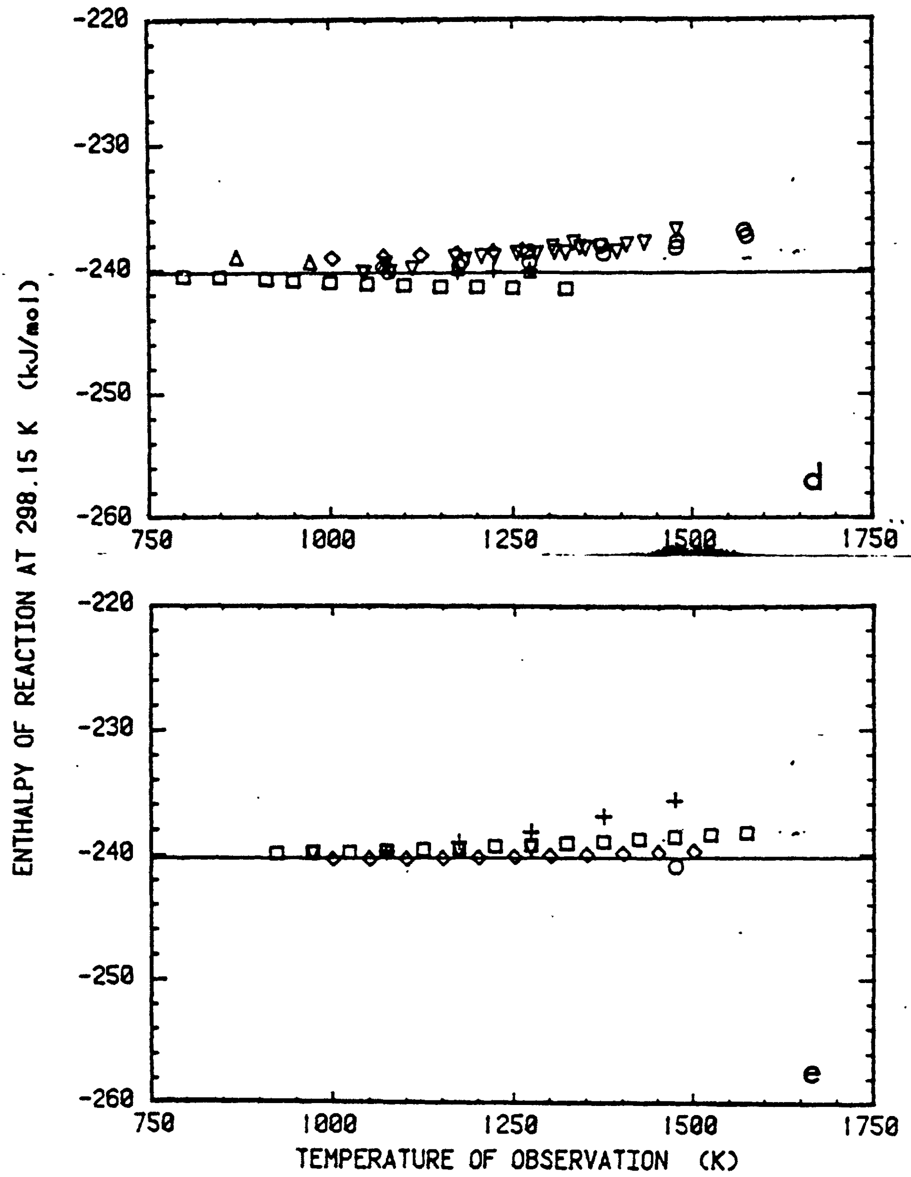
516

Figure A.10.



517

Figure A.18.



518

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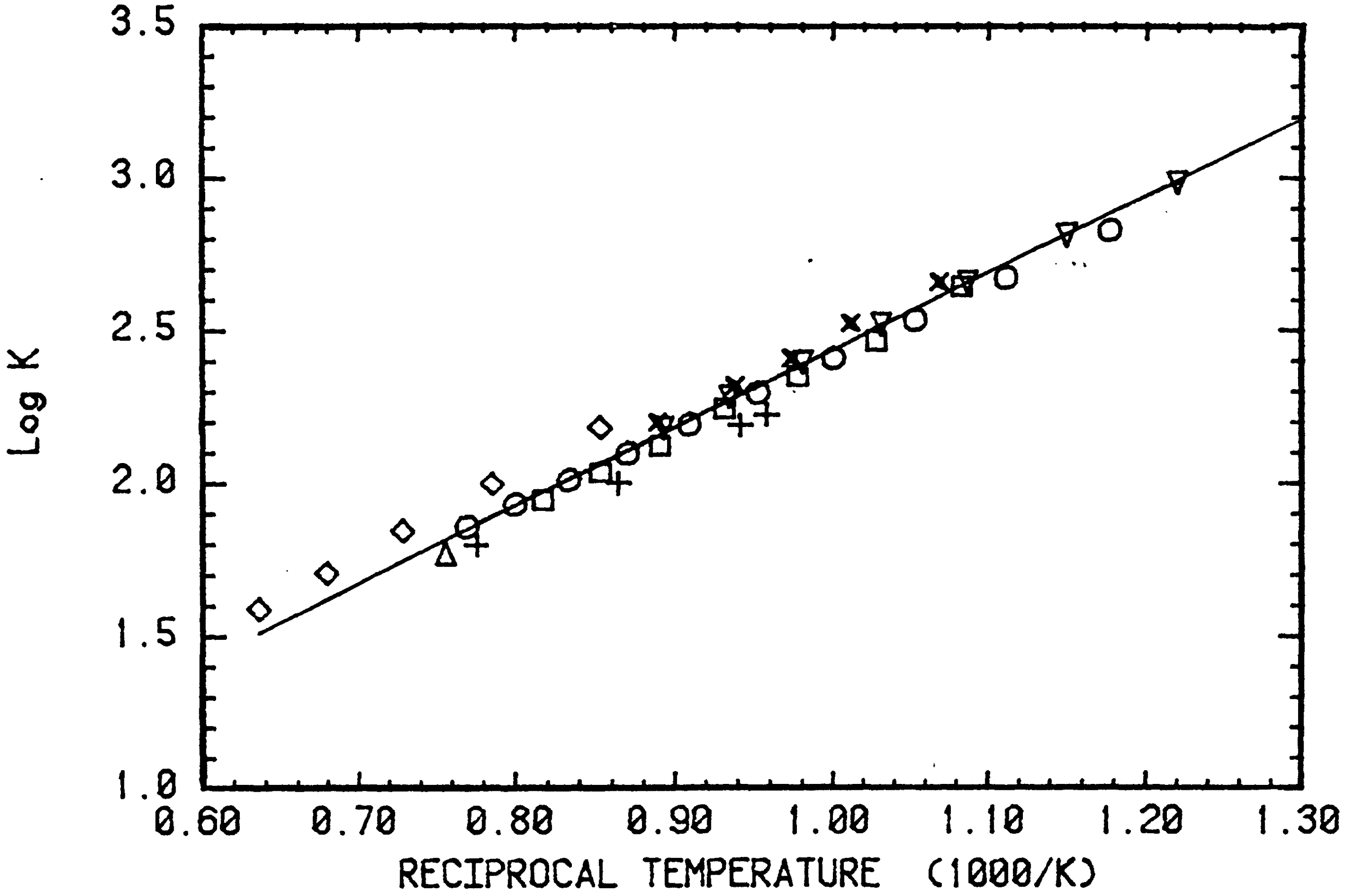
Figure A.11



519

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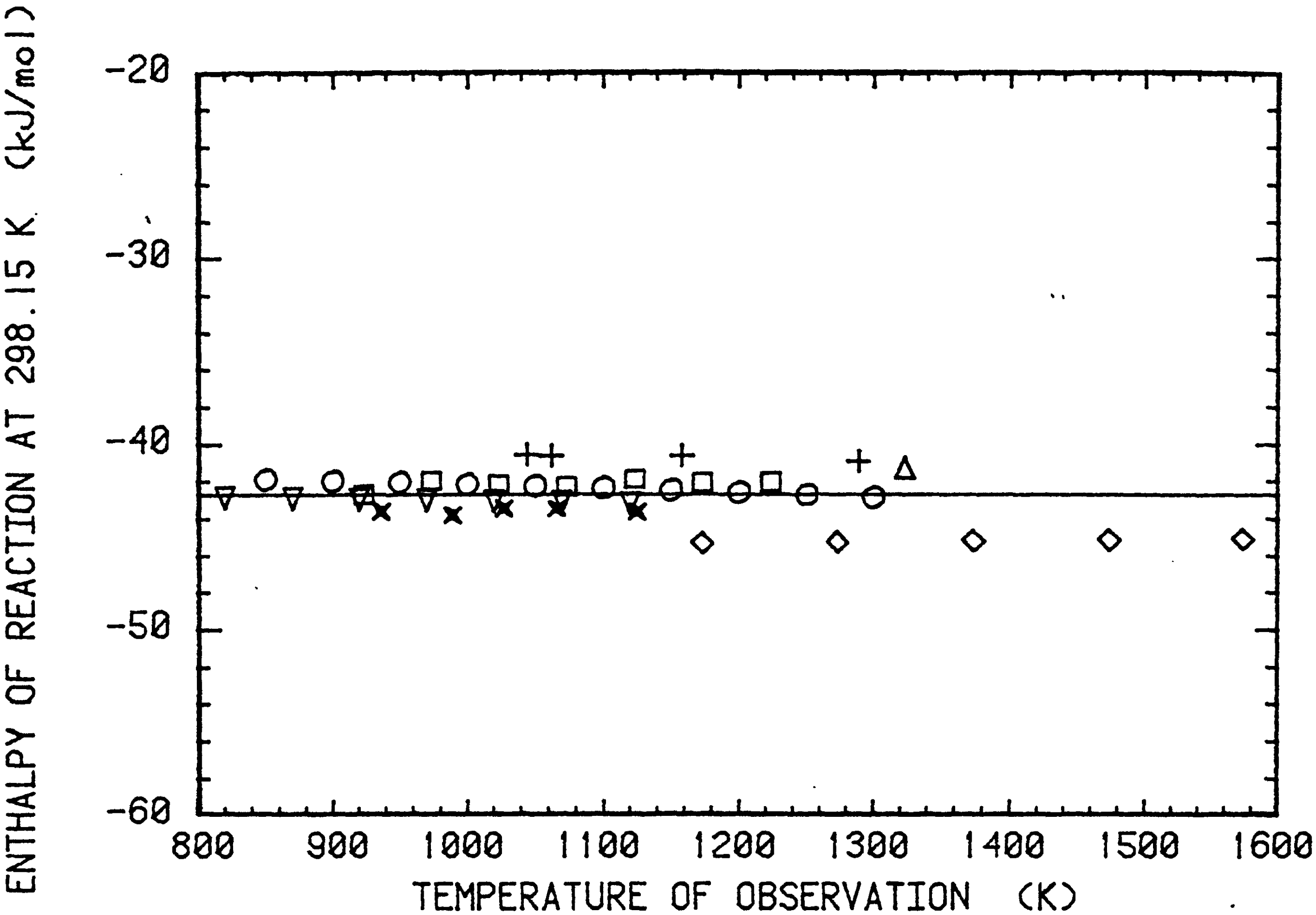
Figure A.12



520

Figure A.13

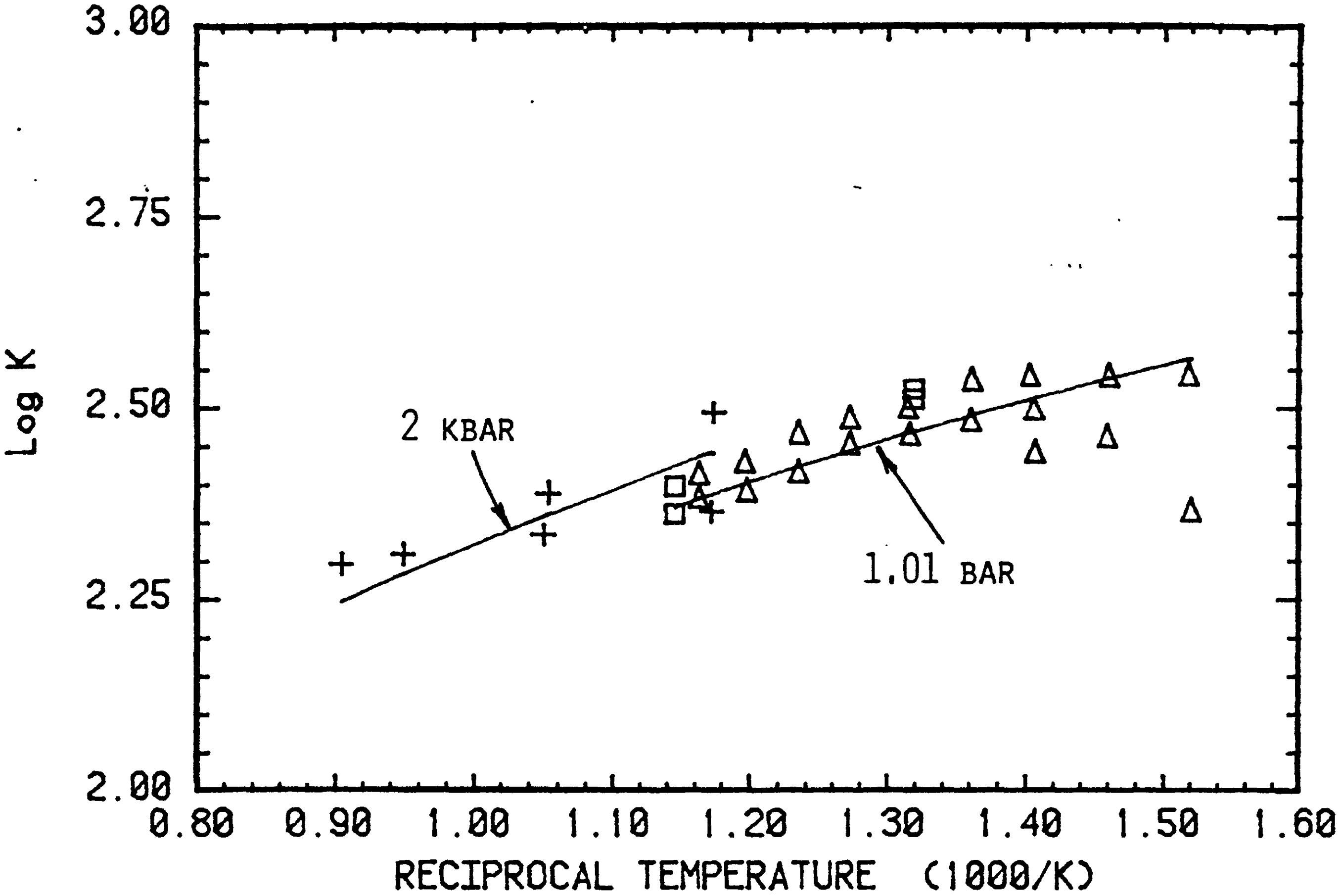

3.00
2.75
2.50
2.25
2.00
Log K
0.80
0.90
1.00
1.10
1.20
1.30
1.40
1.50
1.60
RECIPROCAL TEMPERATURE (1000/K)
2 KBAR
1.01 BAR

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Figure A.14

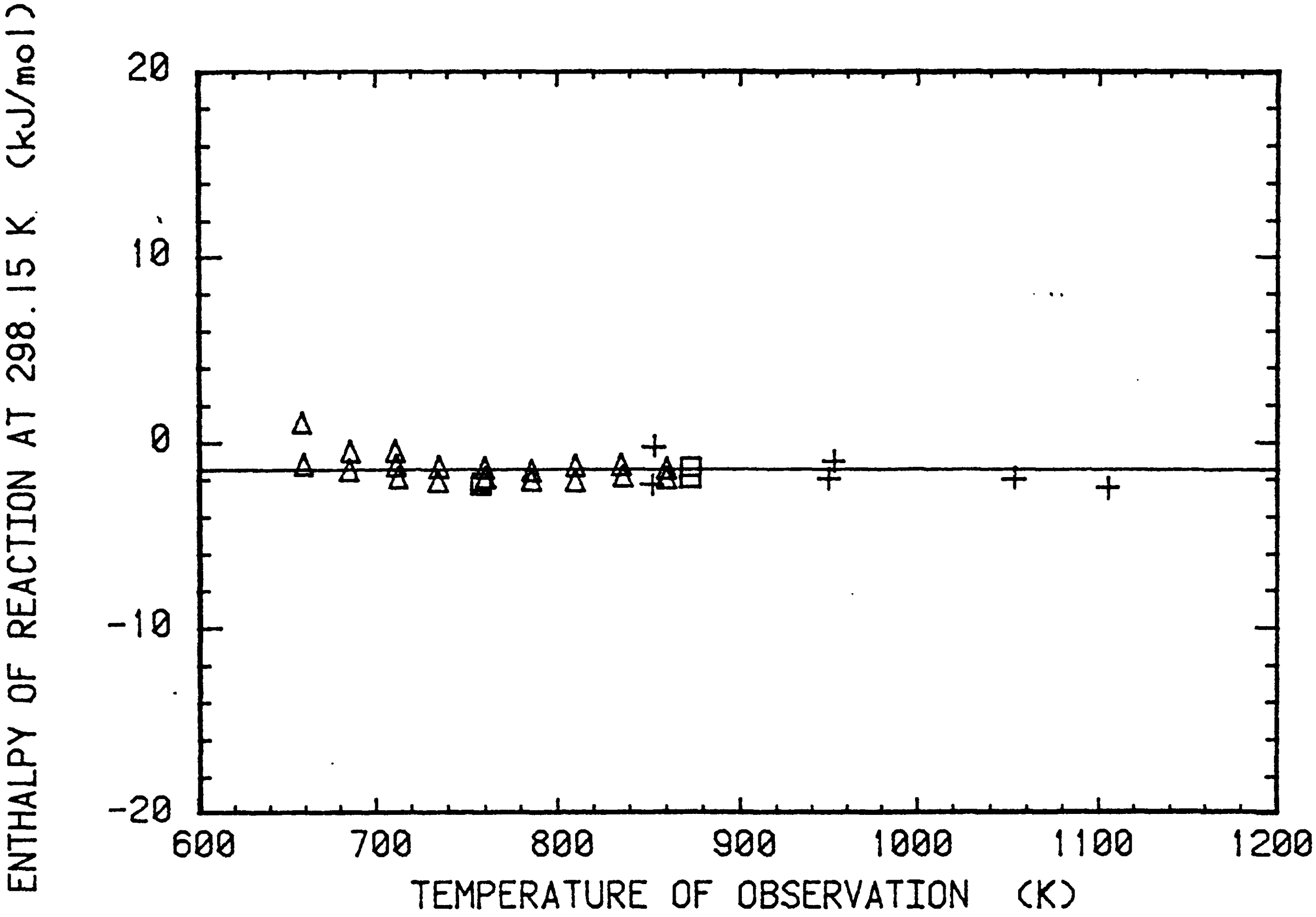
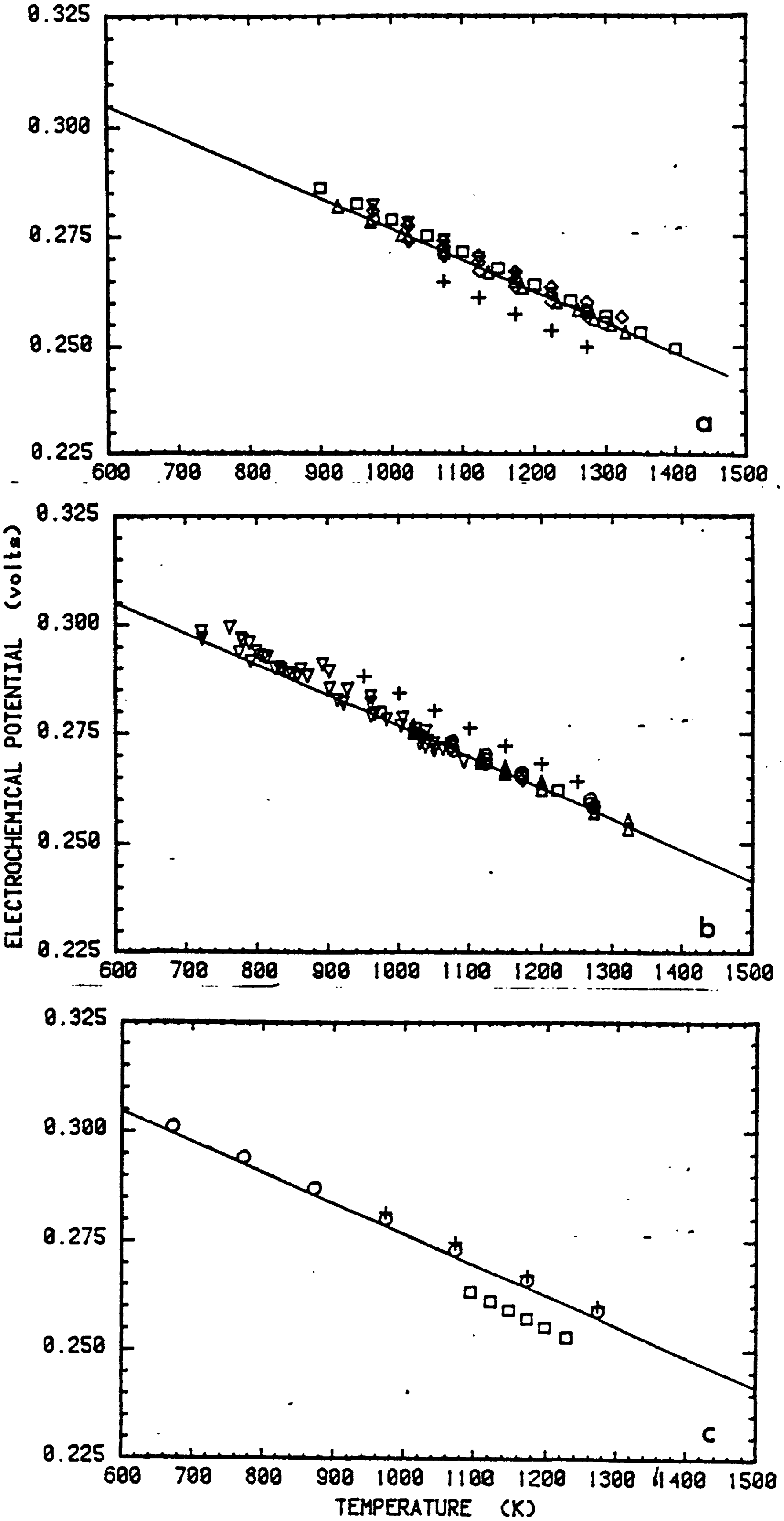
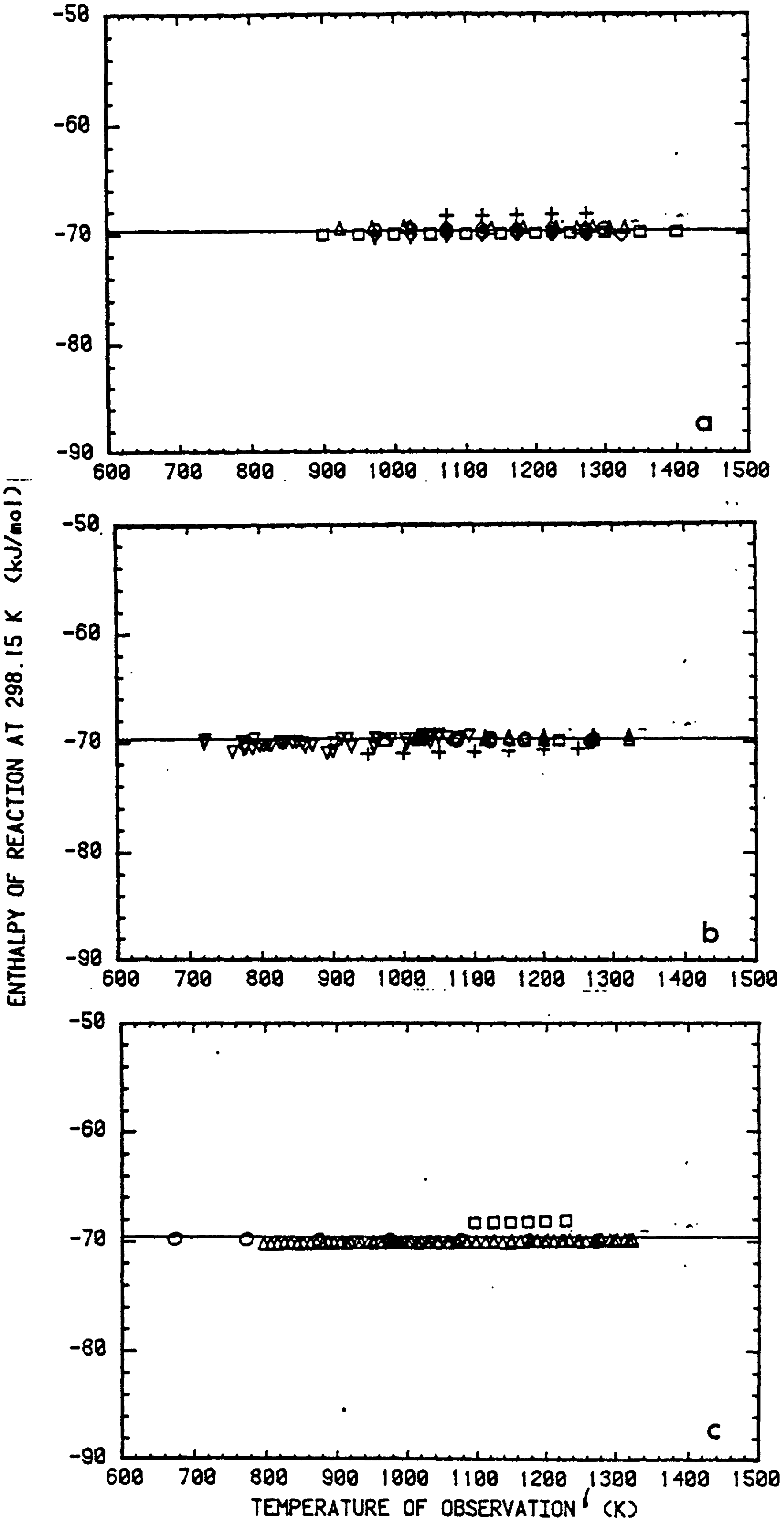


Figure A.15.



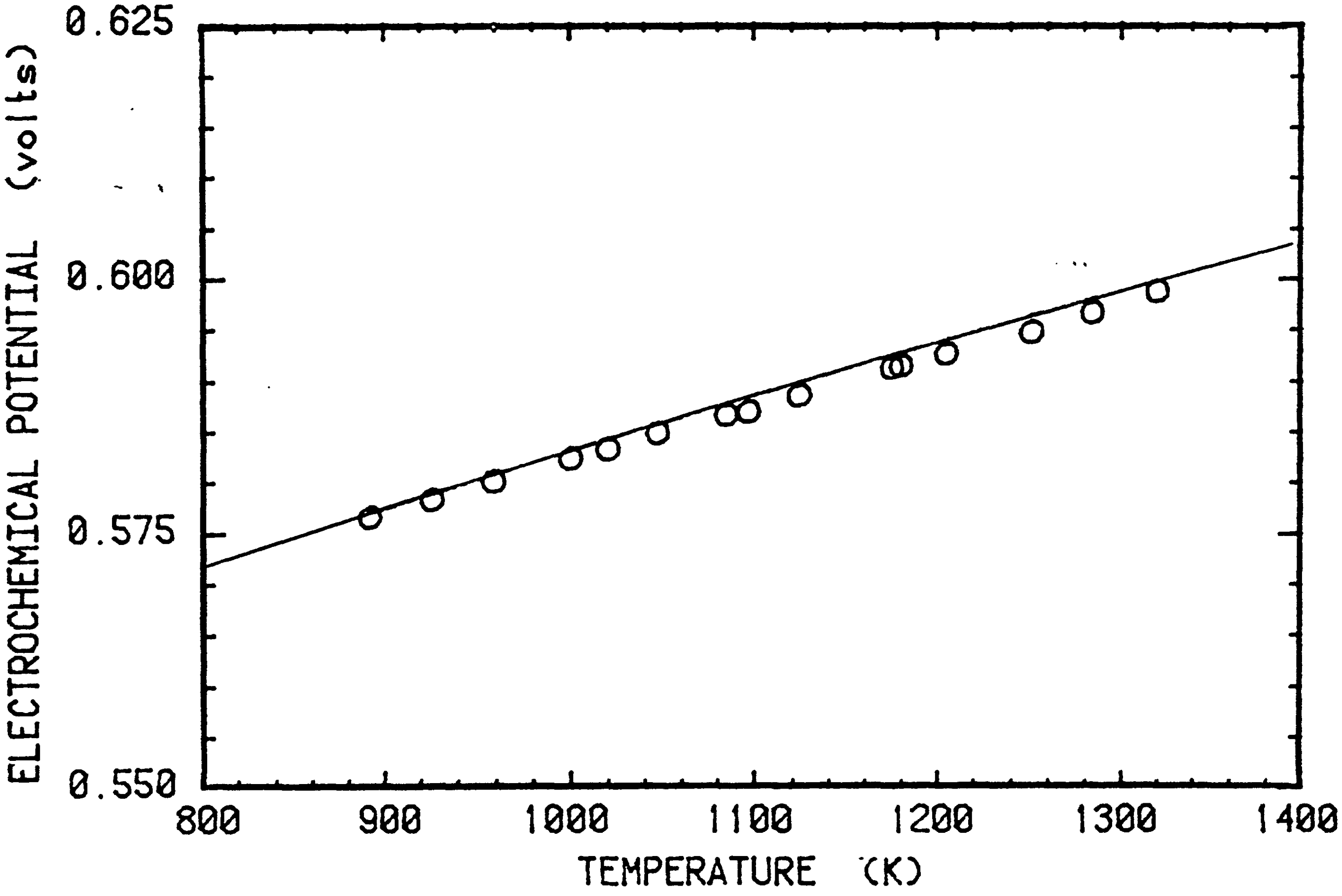
523

Figure A.16.



524

Figure A.17



525

Figure A.18

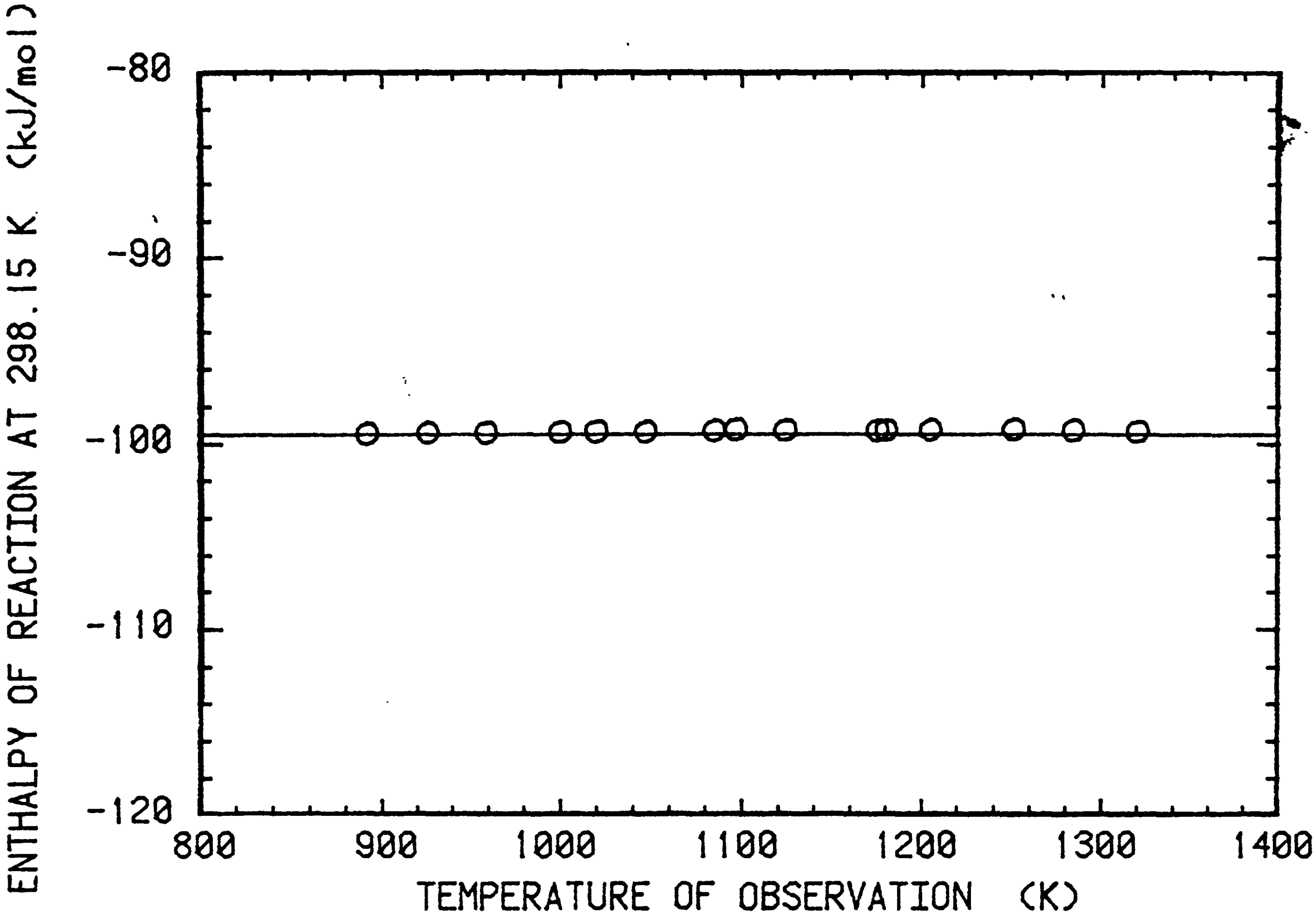

ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
-80
-90
-100
-110
-120
800
900
1000
1100
1200
1300
1400
TEMPERATURE OF OBSERVATION (K)

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Figure A.19,

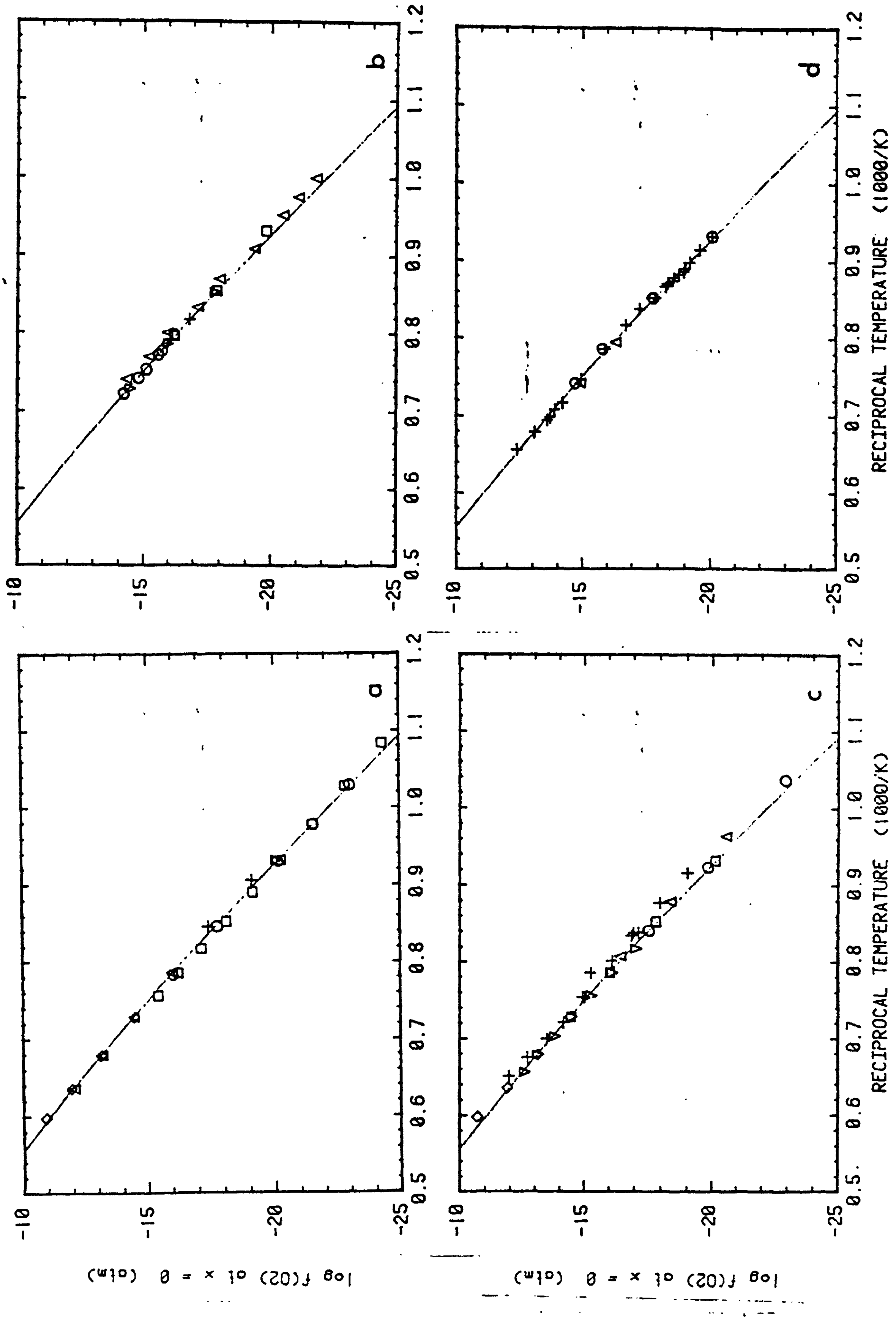

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Figure A.28,

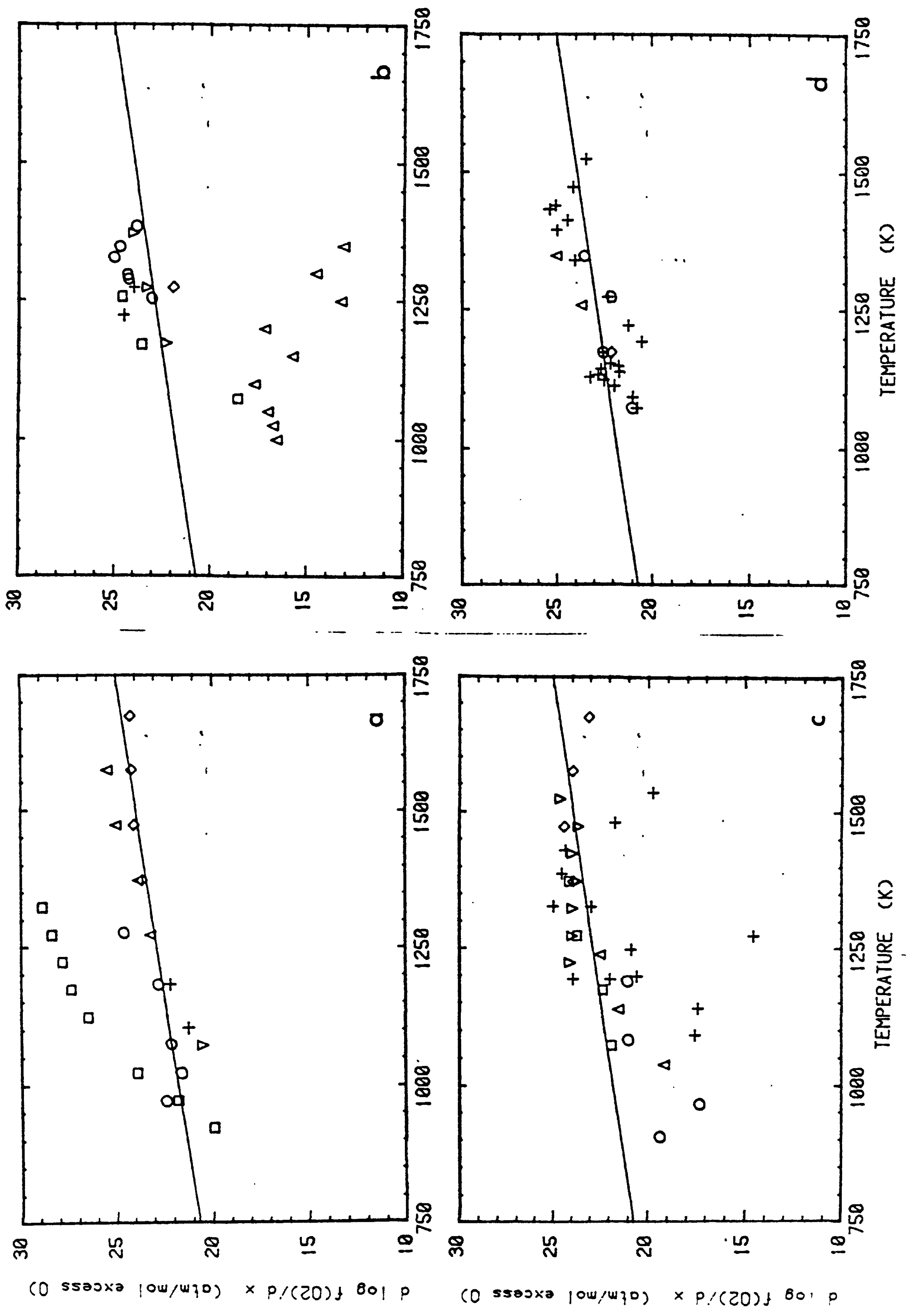

Figure A.21.

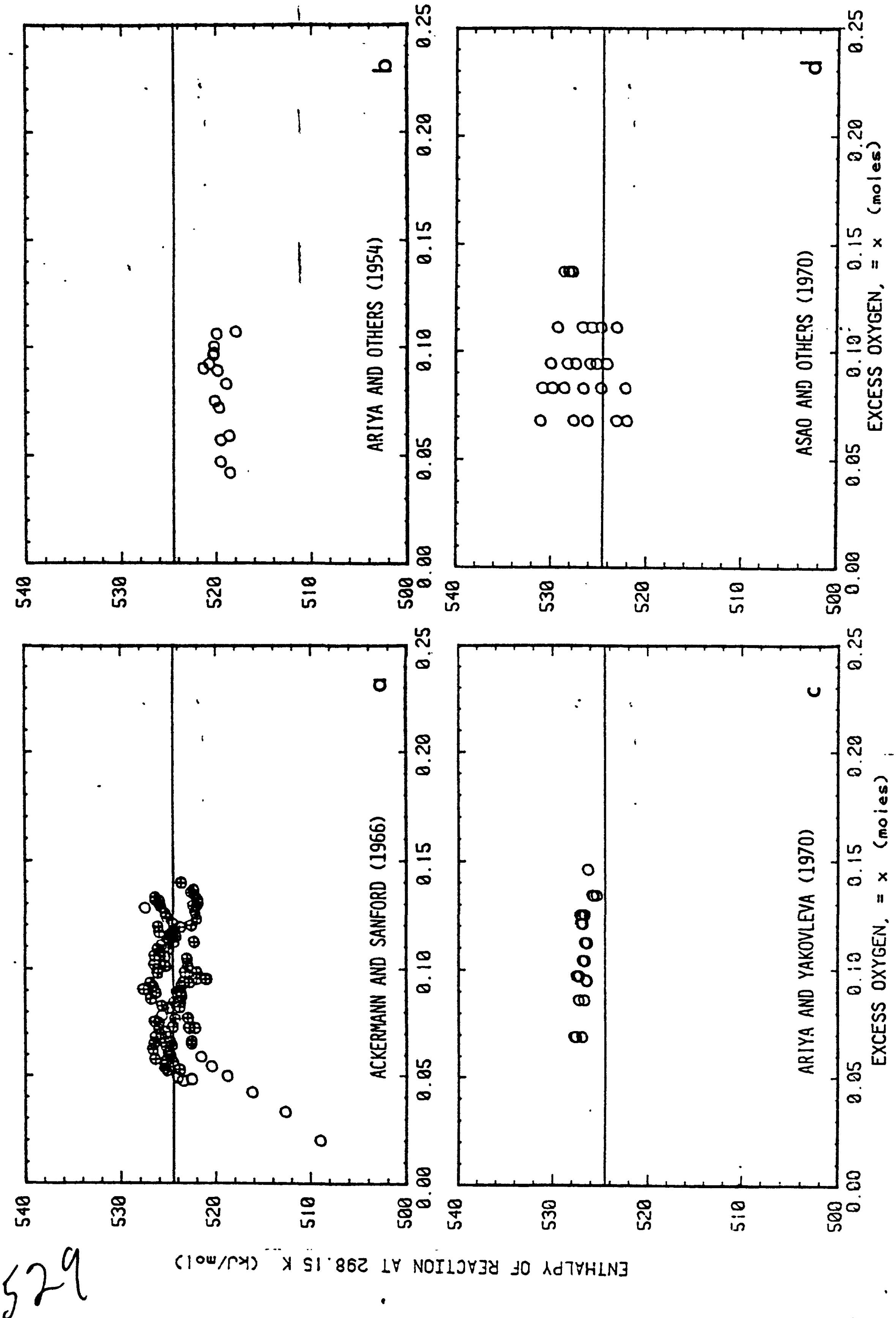
a
ACKERMANN AND SANFORD (1966)
b
ARIYA AND OTHERS (1954)
c
ARIYA AND YAKOVLEVA (1970)
d
ASAO AND OTHERS (1970)
EXCESS OXYGEN, = x (moles)
0.00
0.05
0.10
0.15
0.20
0.25
ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
500
510
520
530
540

Figure A.21.

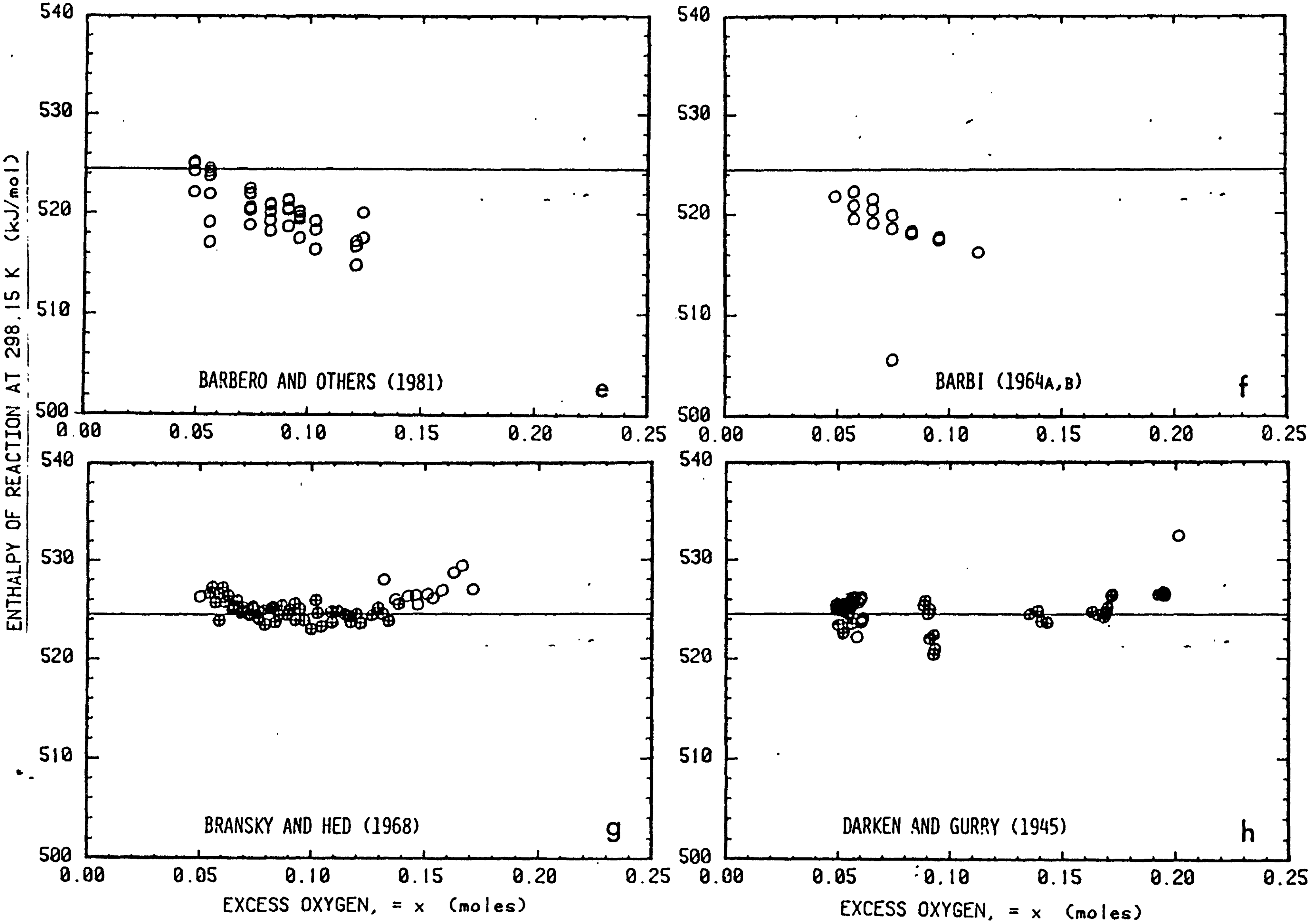
ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
540
530
520
510
500
BARBERO AND OTHERS (1981)
e
BARBI (1964A,B)
f
BRANSKY AND HED (1968)
g
DARKEN AND GURRY (1945)
h
0.00
0.05
0.10
0.15
0.20
0.25
EXCESS OXYGEN, = x (moles)

Figure A.21.

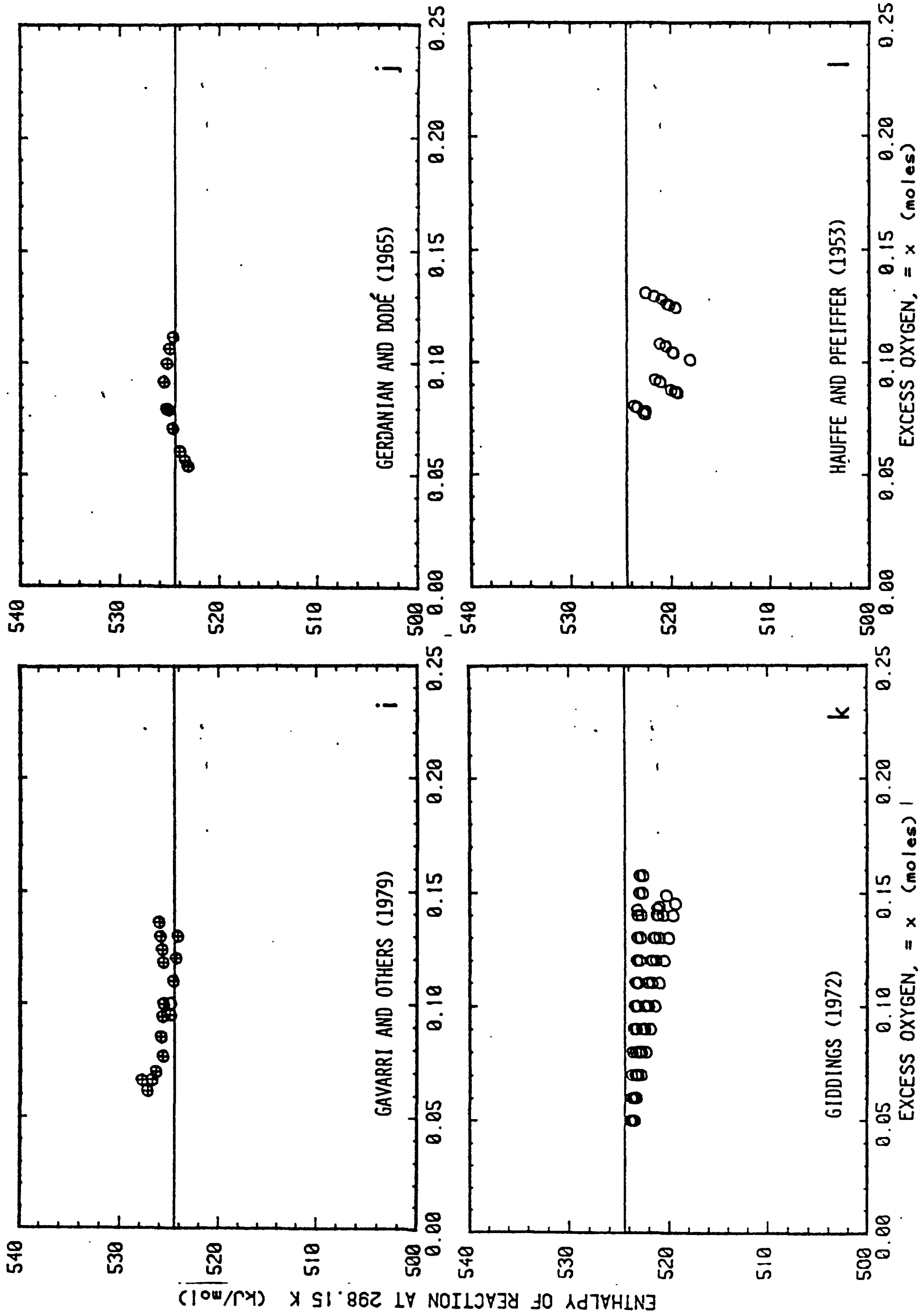
GERDANIAN AND DODÉ (1965)
j
HAUFFE AND PFEIFFER (1953)
l
GAVARRI AND OTHERS (1979)
i
GIDDINGS (1972)
k
ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
EXCESS OXYGEN, = x (moles)
540
530
520
510
500
0.00
0.05
0.10
0.15
0.20
0.25

Figure A.21.

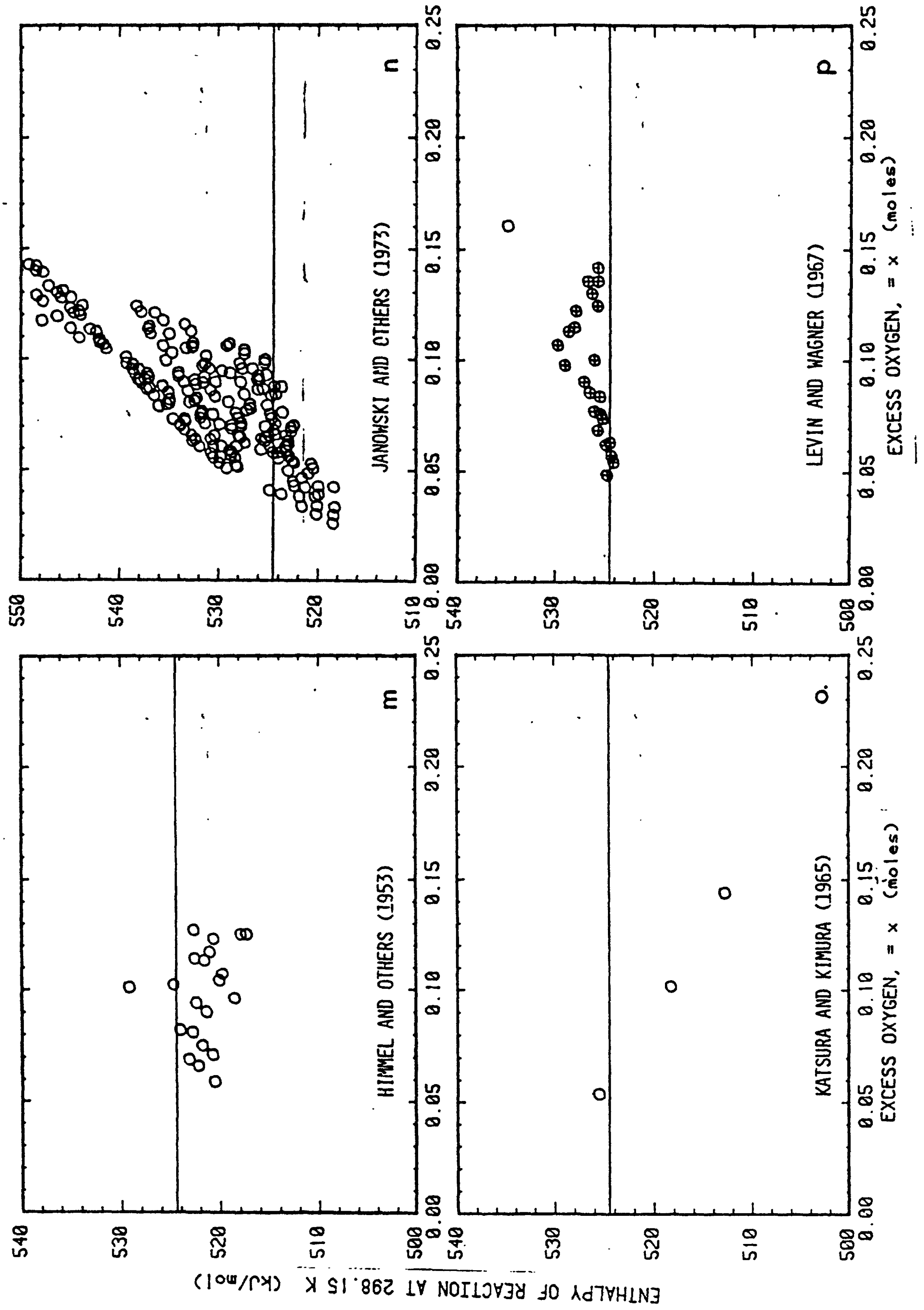
n
JANOWSKI AND OTHERS (1973)
m
HIMMEL AND OTHERS (1953)
p
LEVIN AND WAGNER (1967)
o
KATSURA AND KIMURA (1965)
EXCESS OXYGEN, = x (moles)
ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
0.00
0.05
0.10
0.15
0.20
0.25
550
540
530
520
510
500

Figure A.21.

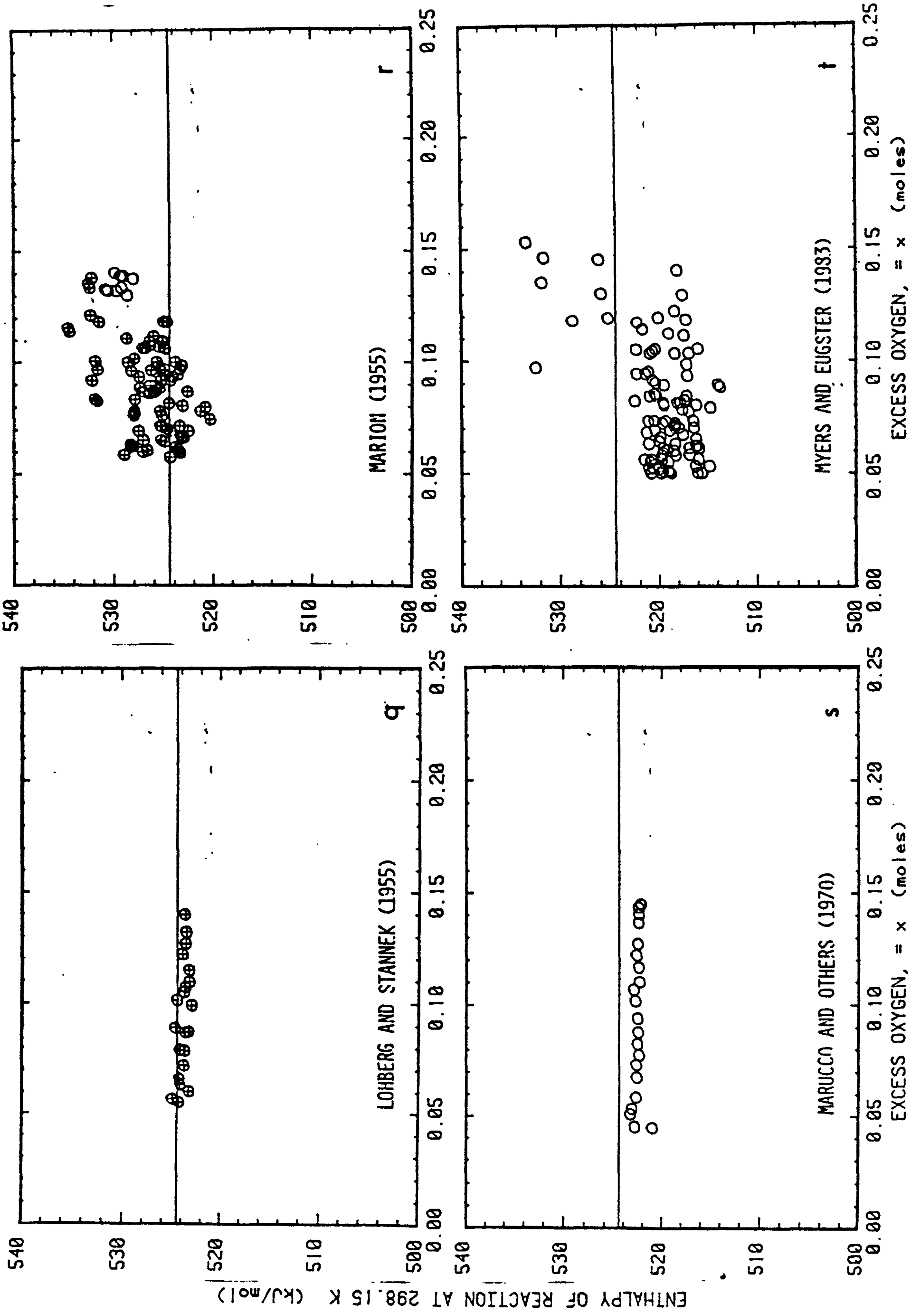
r
MARION (1955)
t
MYERS AND EUGSTER (1983)
q
LOHBERG AND STANNEK (1955)
s
MARUCCO AND OTHERS (1970)
ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
EXCESS OXYGEN, = x (moles)
540
530
520
510
500
0.00
0.05
0.10
0.15
0.20
0.25

Figure A.21.

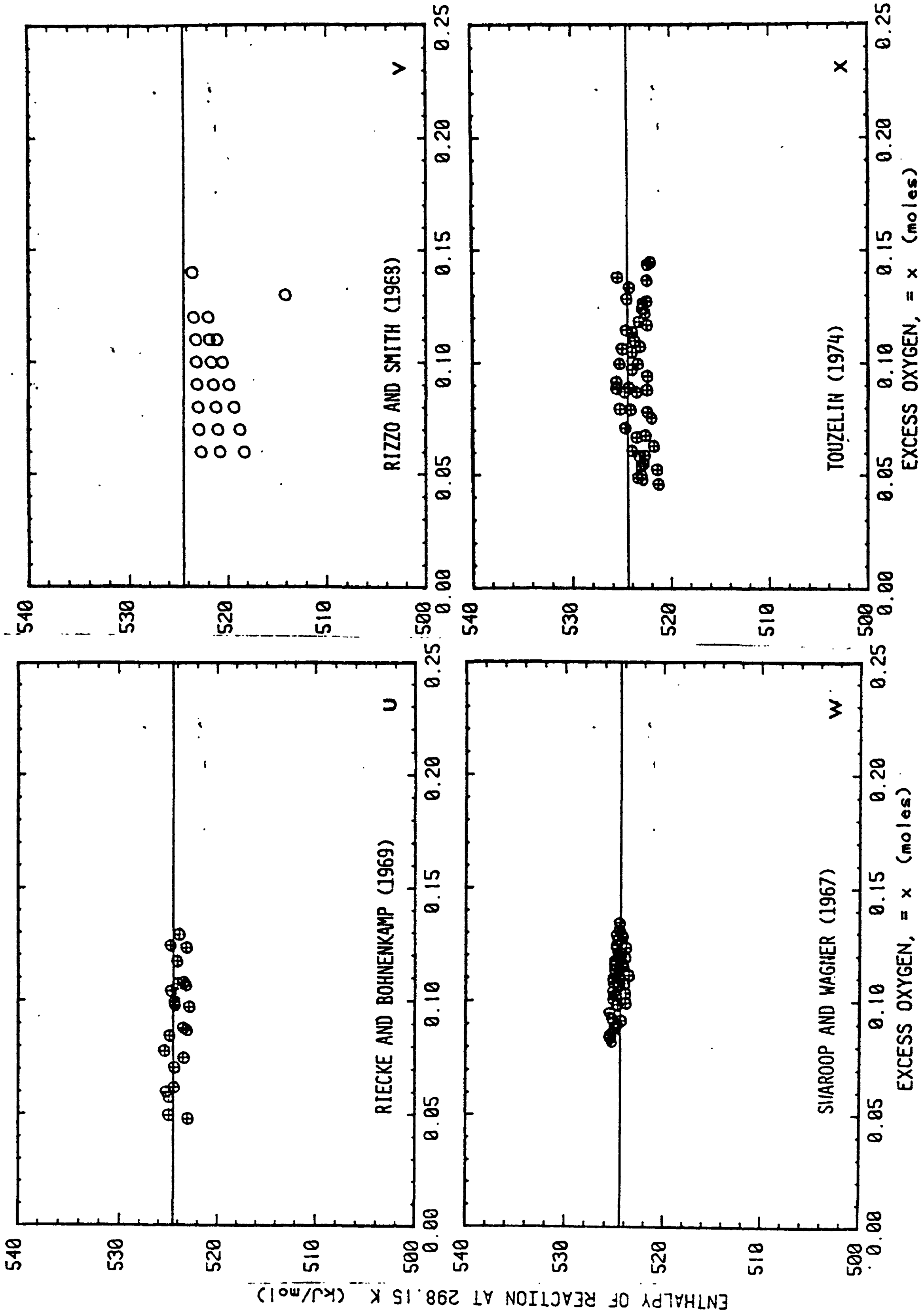
V
RIZZO AND SMITH (1968)
X
TOUZELIN (1974)
U
RIECKE AND BOHNENKAMP (1969)
W
SHAROOP AND WAGNER (1967)
0.00
0.05
0.10
0.15
0.20
0.25
EXCESS OXYGEN, = x (moles)
540
530
520
510
500
ENTHALPY OF REACTION AT 298.15 K (kJ/mol)

Figure A.21.

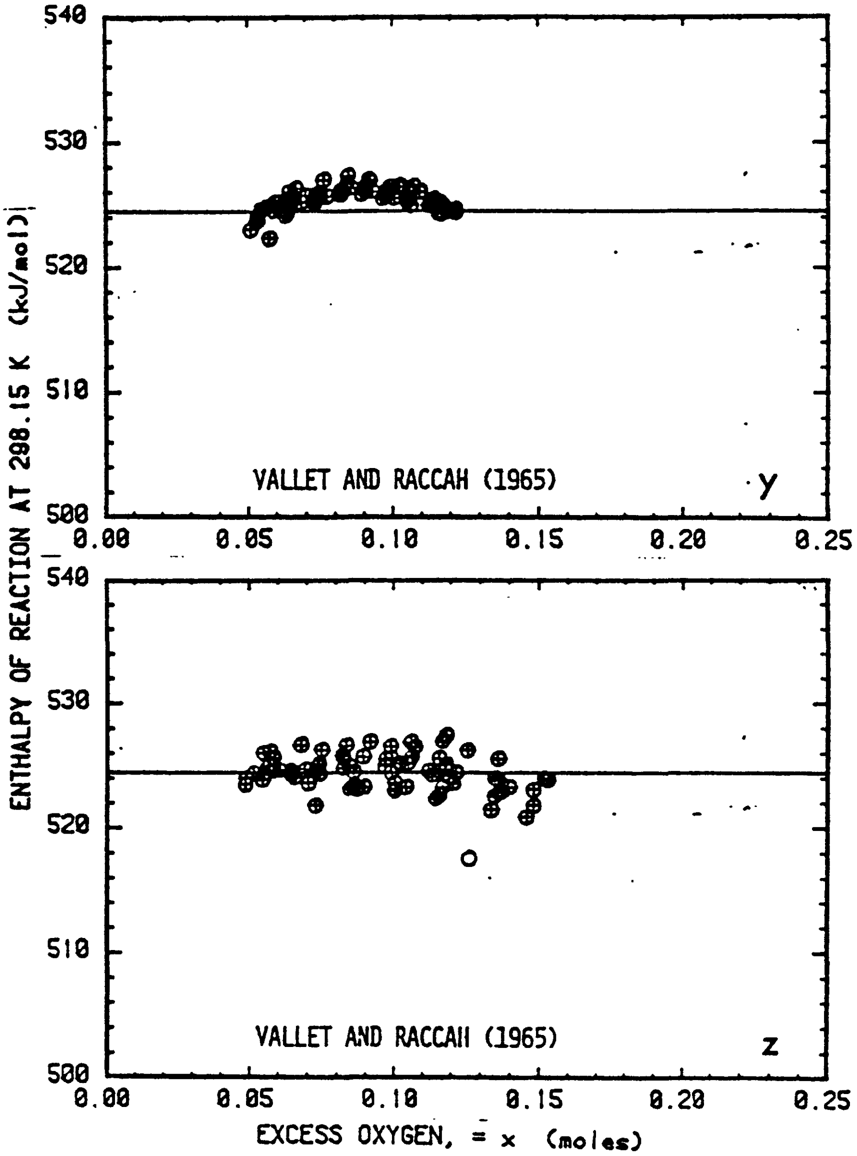
540
530
520
510
500
ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
VALLET AND RACCAH (1965)
y
0.00
0.05
0.10
0.15
0.20
0.25
540
530
520
510
500
VALLET AND RACCAH (1965)
z
0.00
0.05
0.10
0.15
0.20
0.25
EXCESS OXYGEN, = x (moles)

Figure A.22.

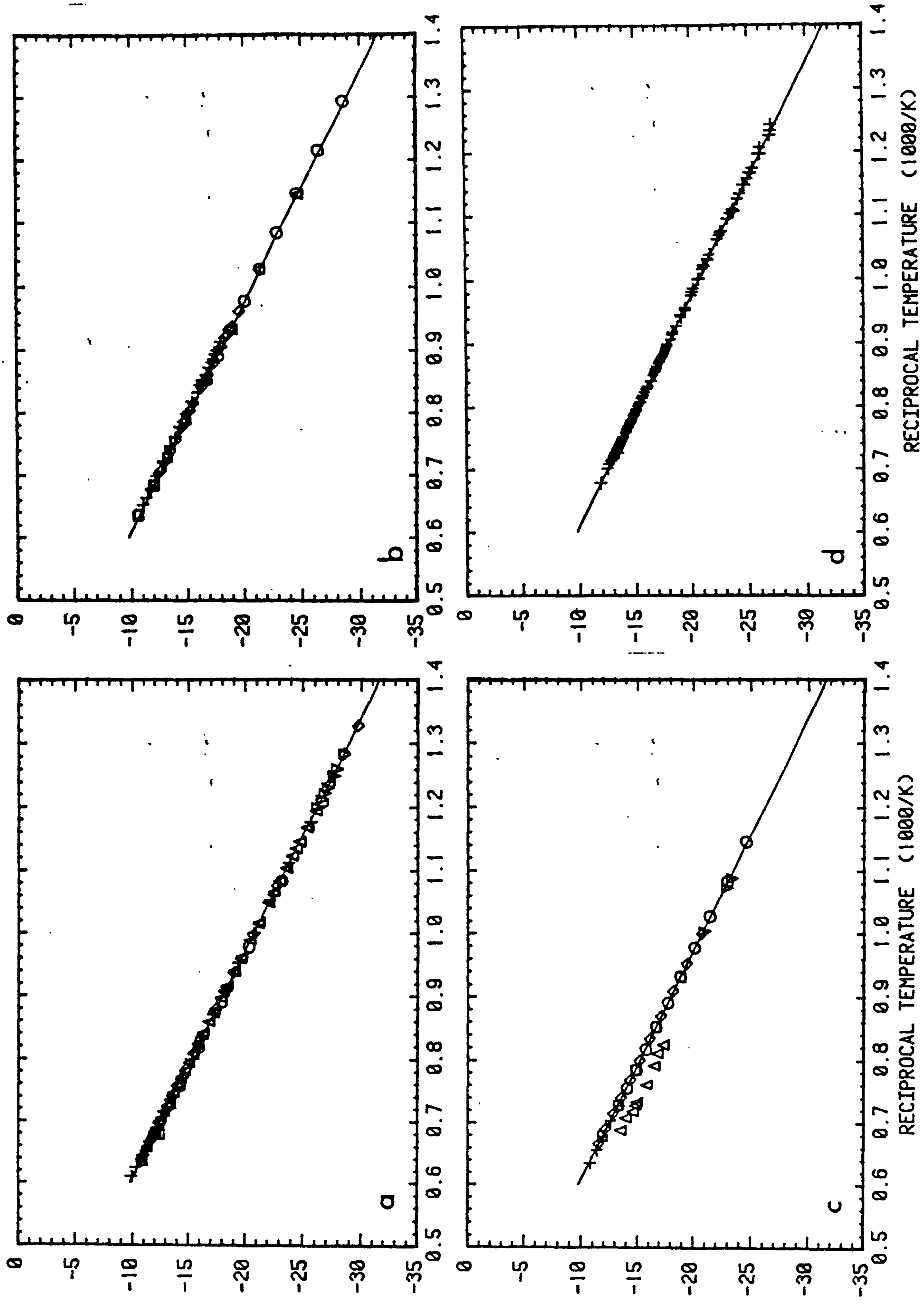
a
b
c
d
Log K
0
-5
-10
-15
-20
-25
-30
-35
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
RECIPROCAL TEMPERATURE (1000/K)

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Figure A.23.

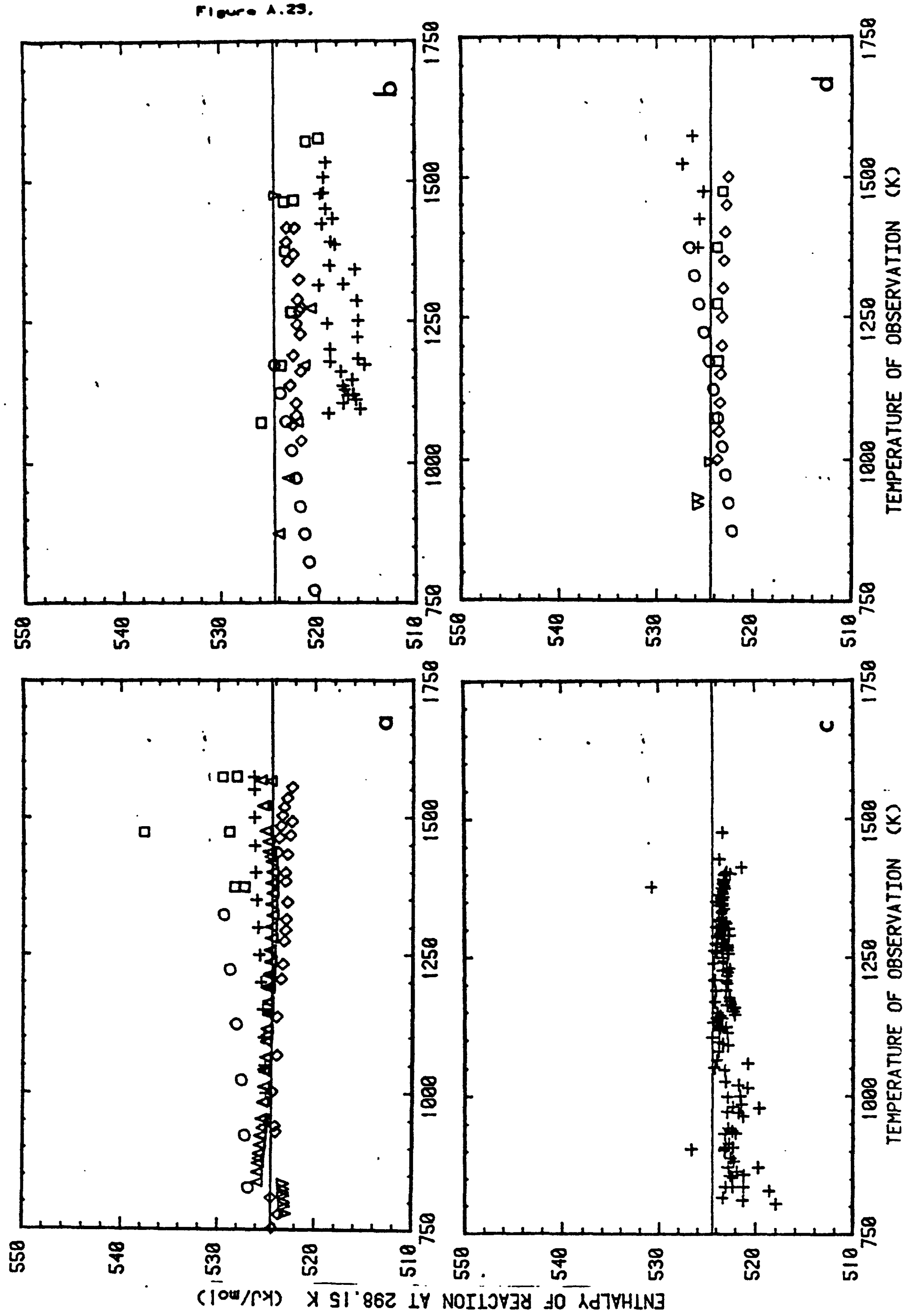
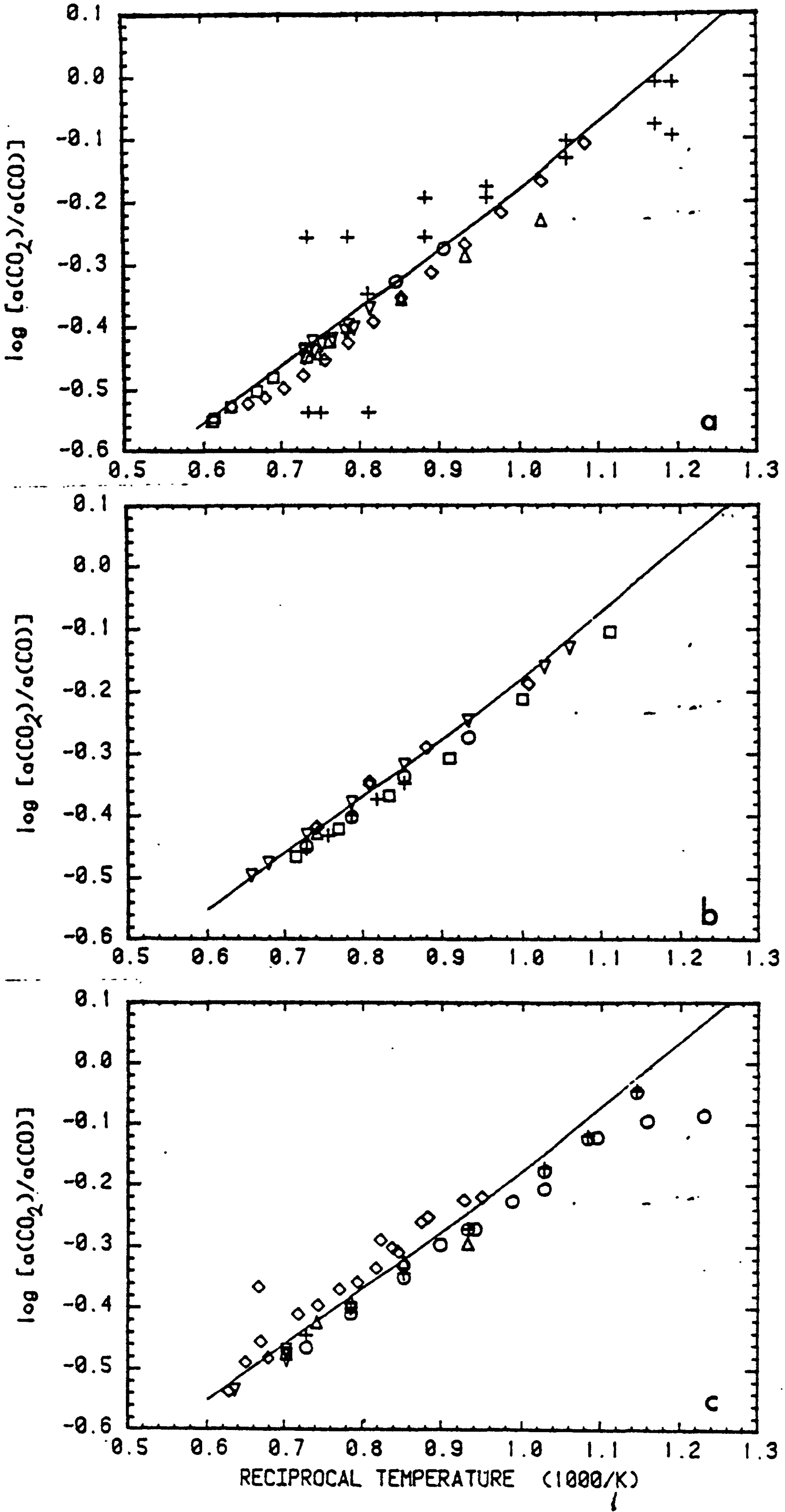
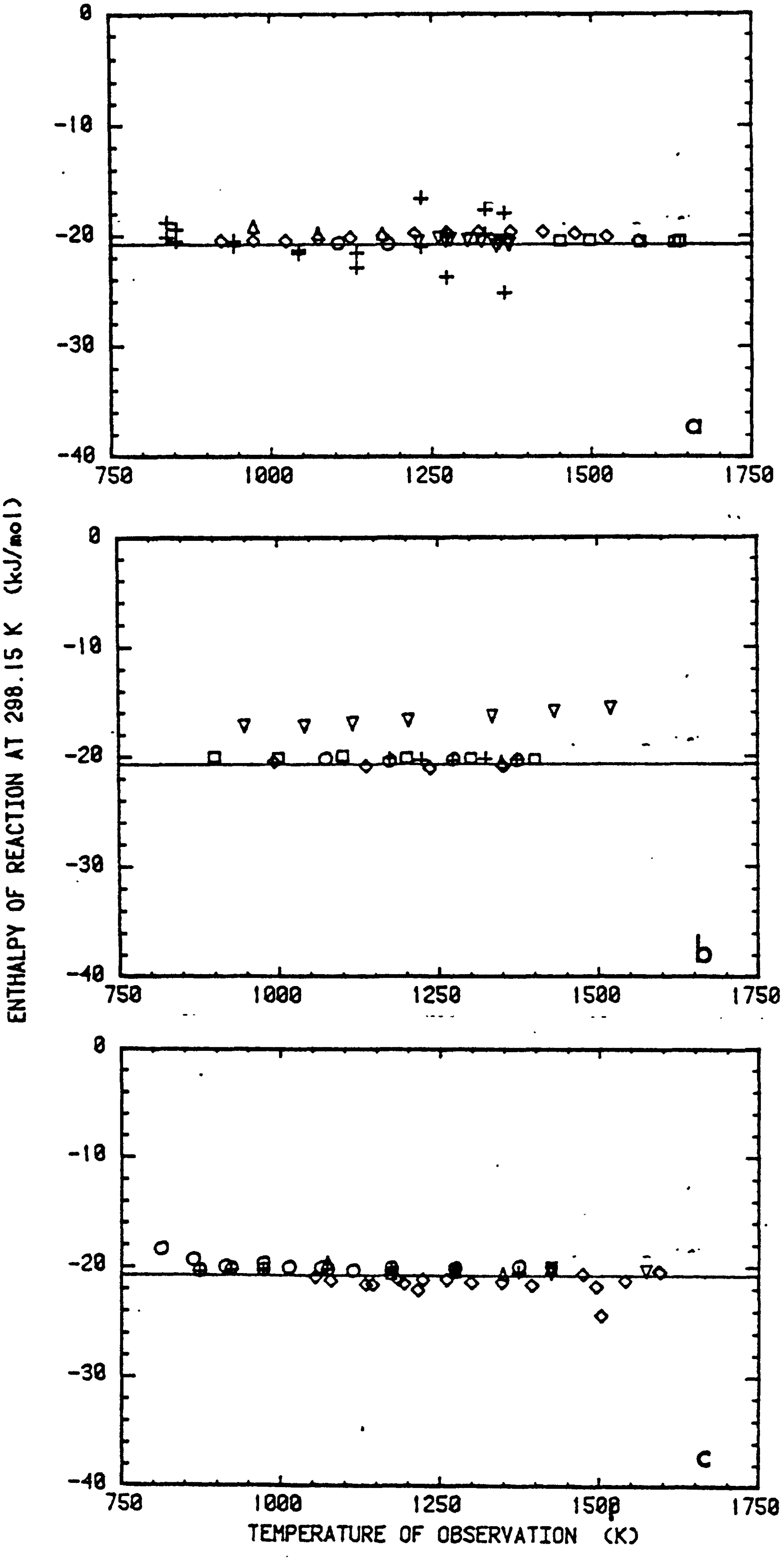


Figure A.24.



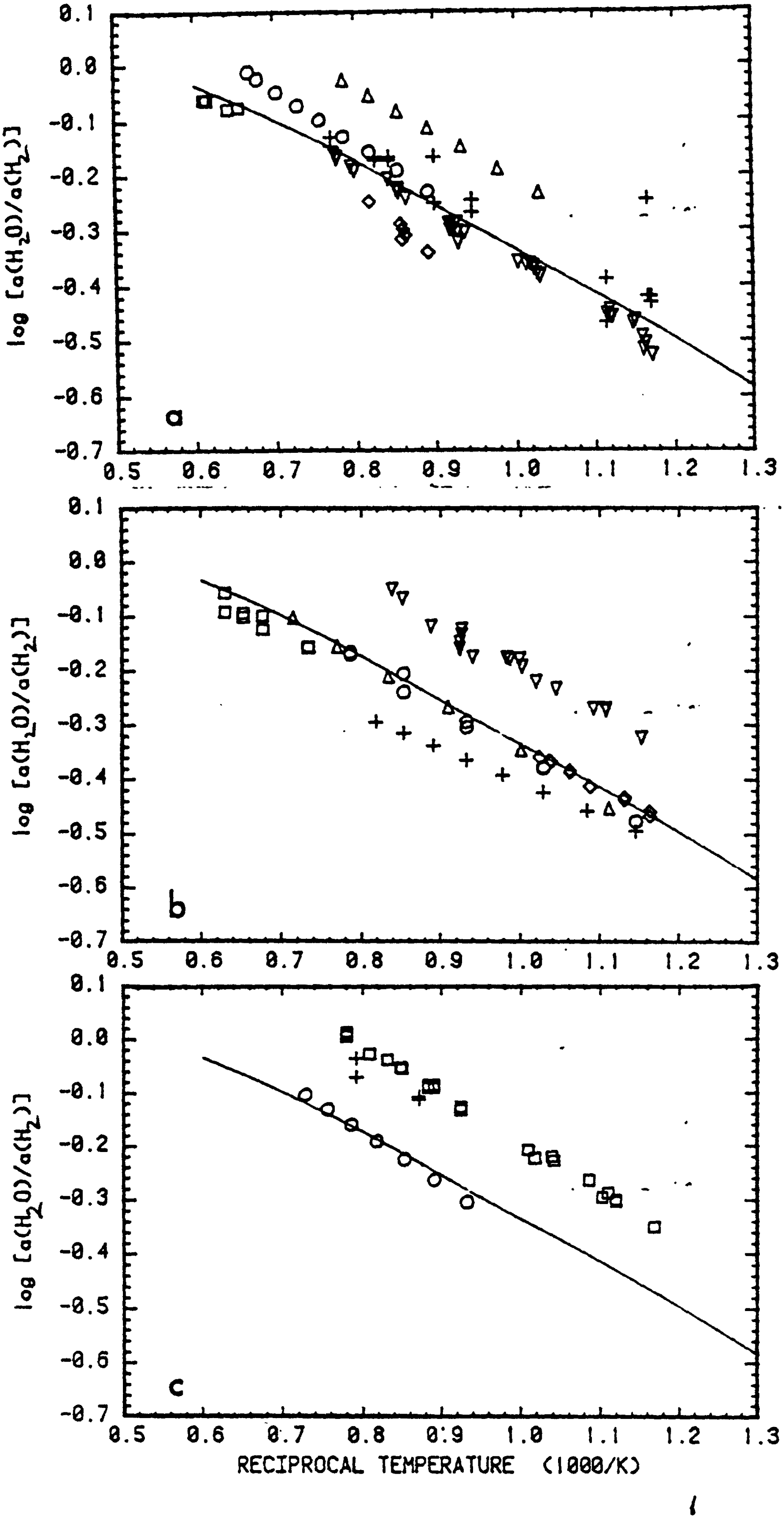
538

Figure A.25.



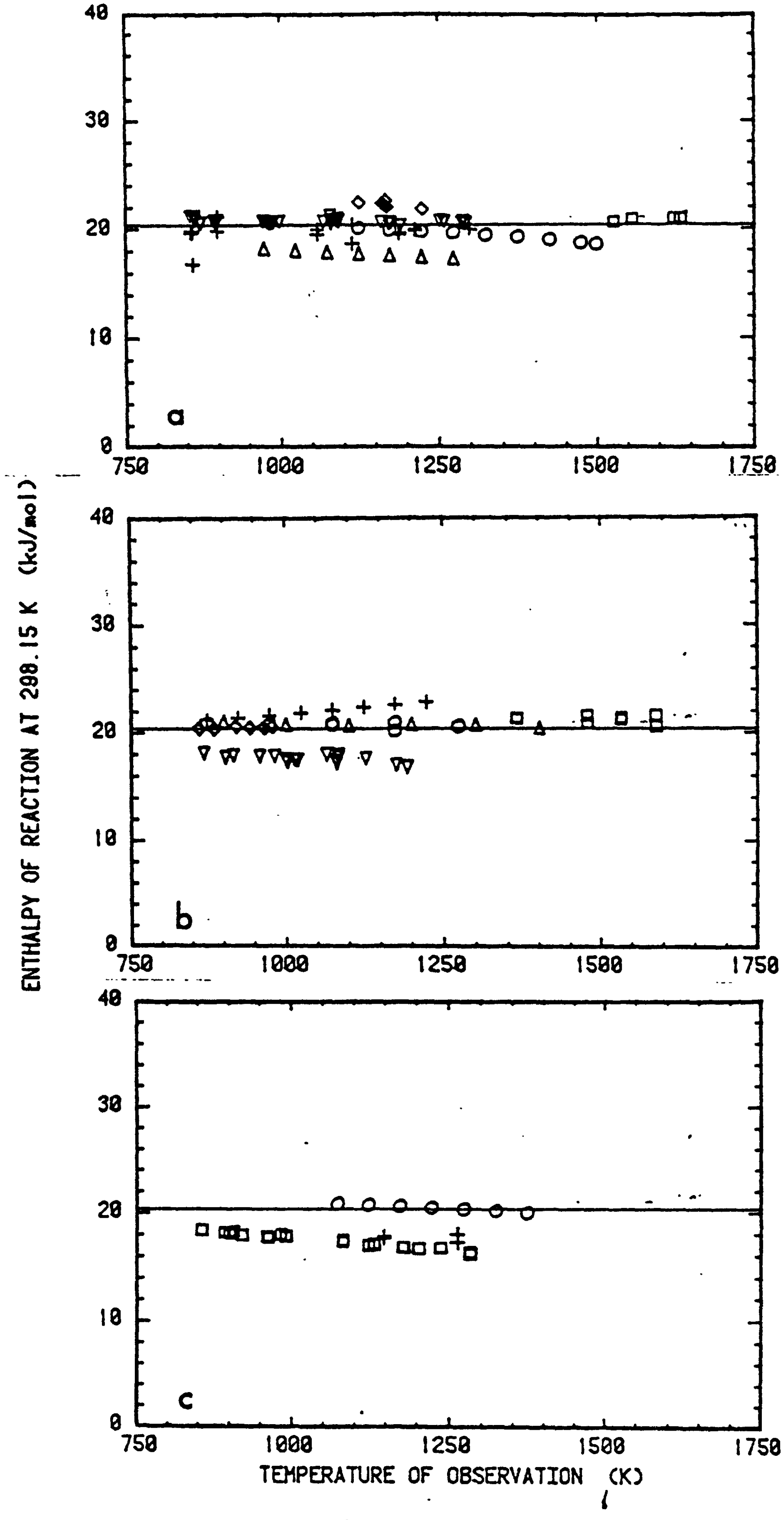
539

Figure A.28.



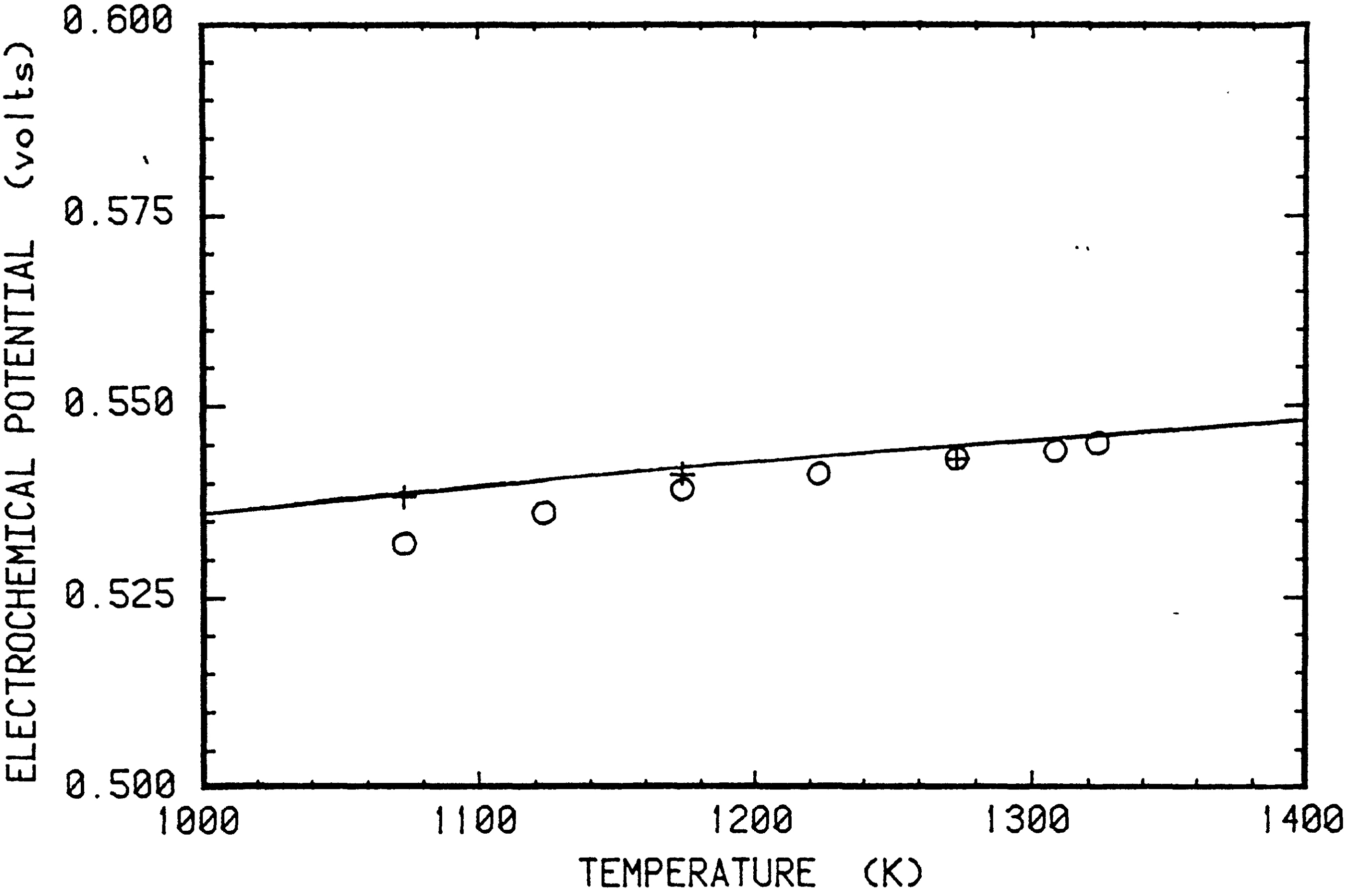
a
b
c
log [a(H_2O)/a(H_2)]
0.1
0.0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
-0.7
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
RECIPROCAL TEMPERATURE (1000/K)

Figure A.27.



541

Figure A.28



542

Figure A.29

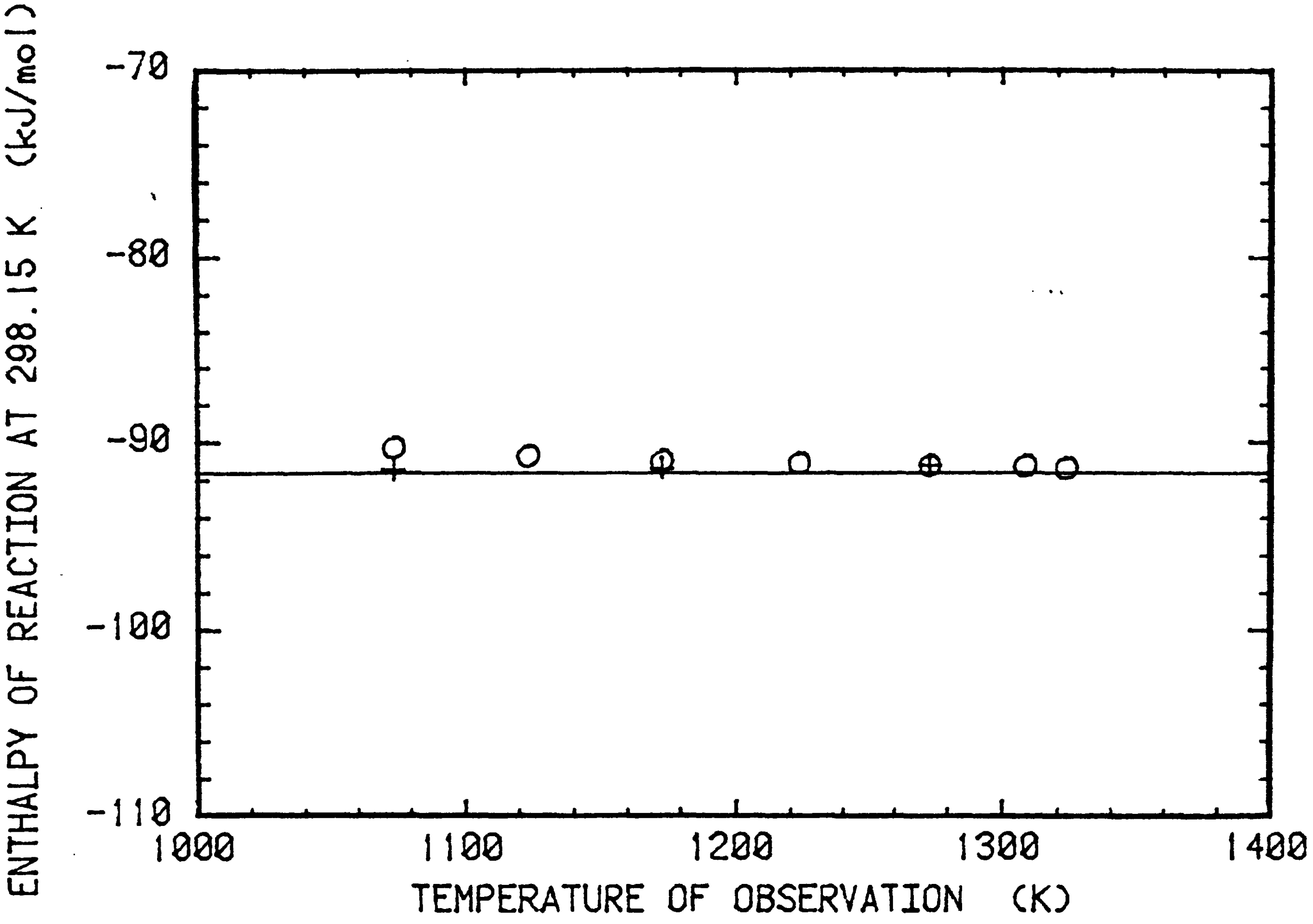

ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
-70
-80
-90
-100
-110
1000
1100
1200
1300
1400
TEMPERATURE OF OBSERVATION (K)

Figure A.30.

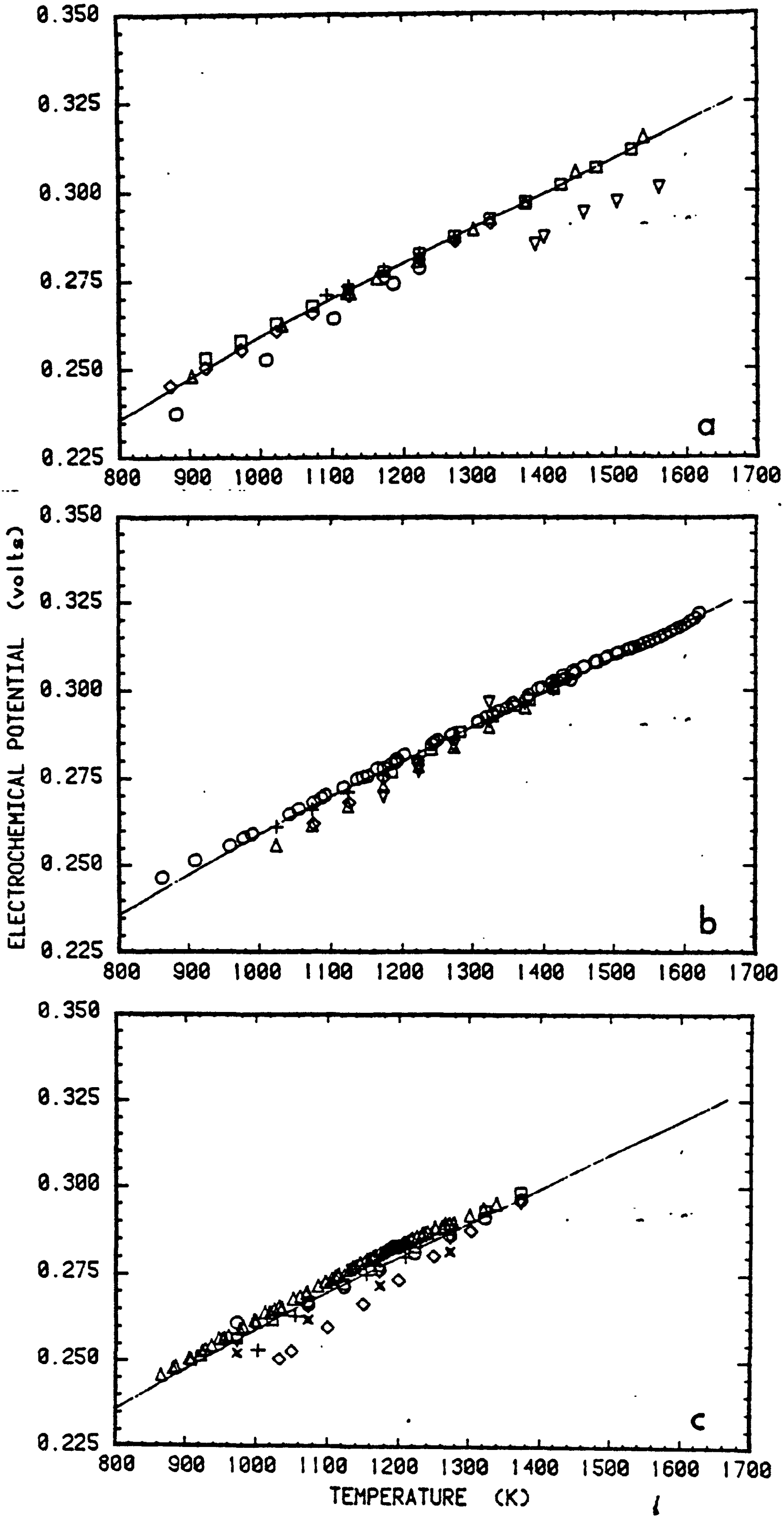
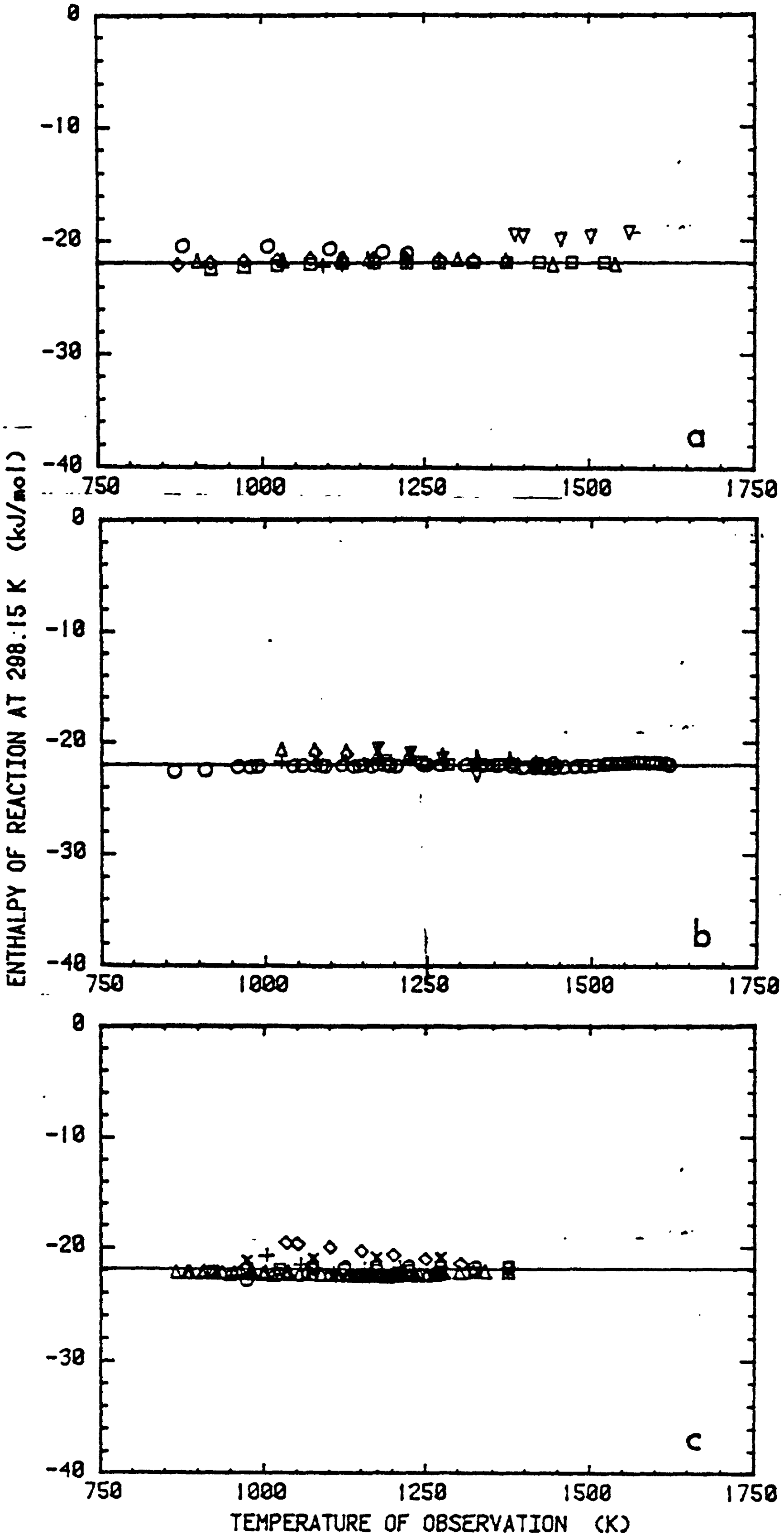

0.350
0.325
0.300
0.275
0.250
0.225
800
900
1000
1100
1200
1300
1400
1500
1600
1700
a
b
c
ELECTROCHEMICAL POTENTIAL (volts)
TEMPERATURE (K)

Figure A.31.



545

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Figure A.32

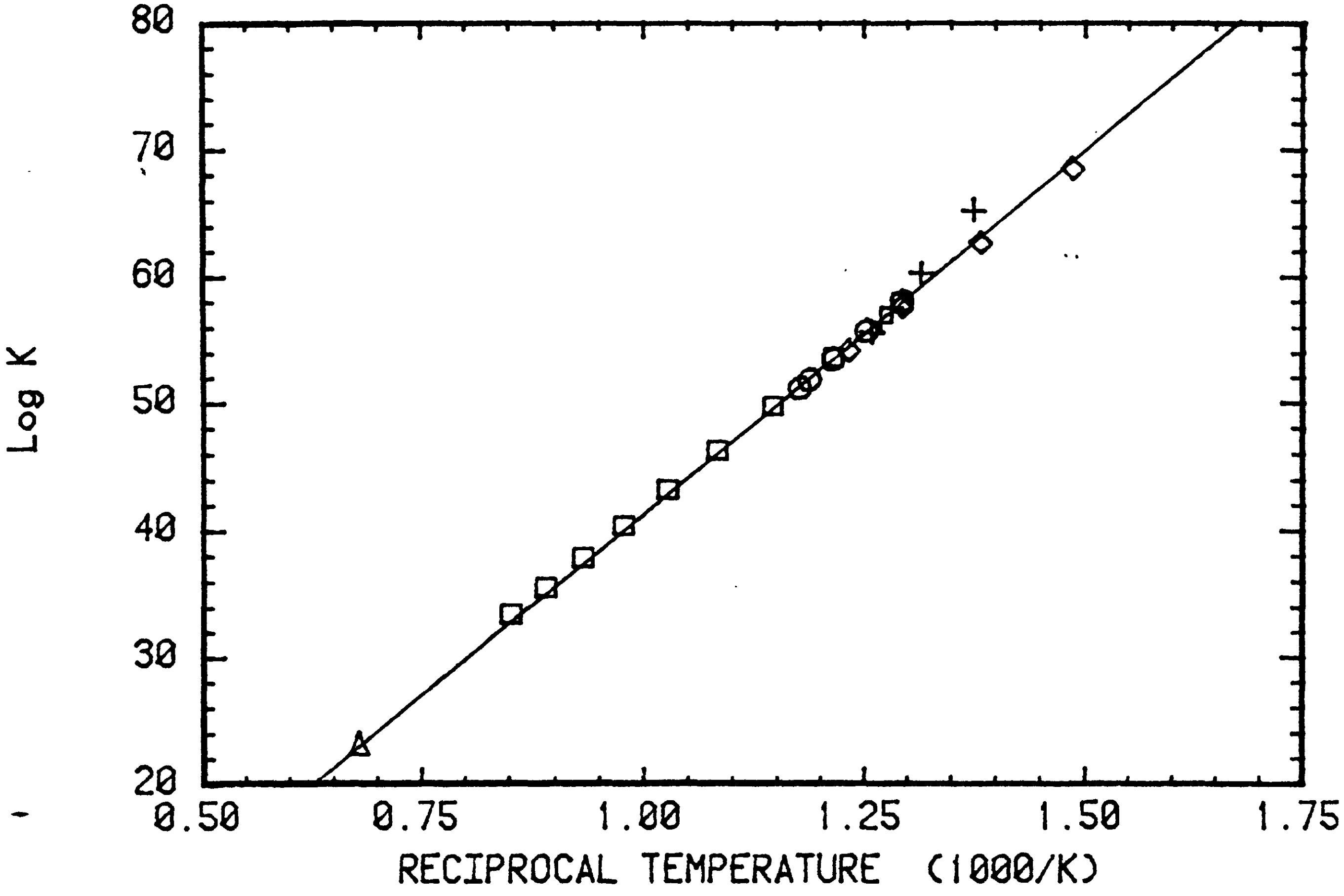

Figure A.33

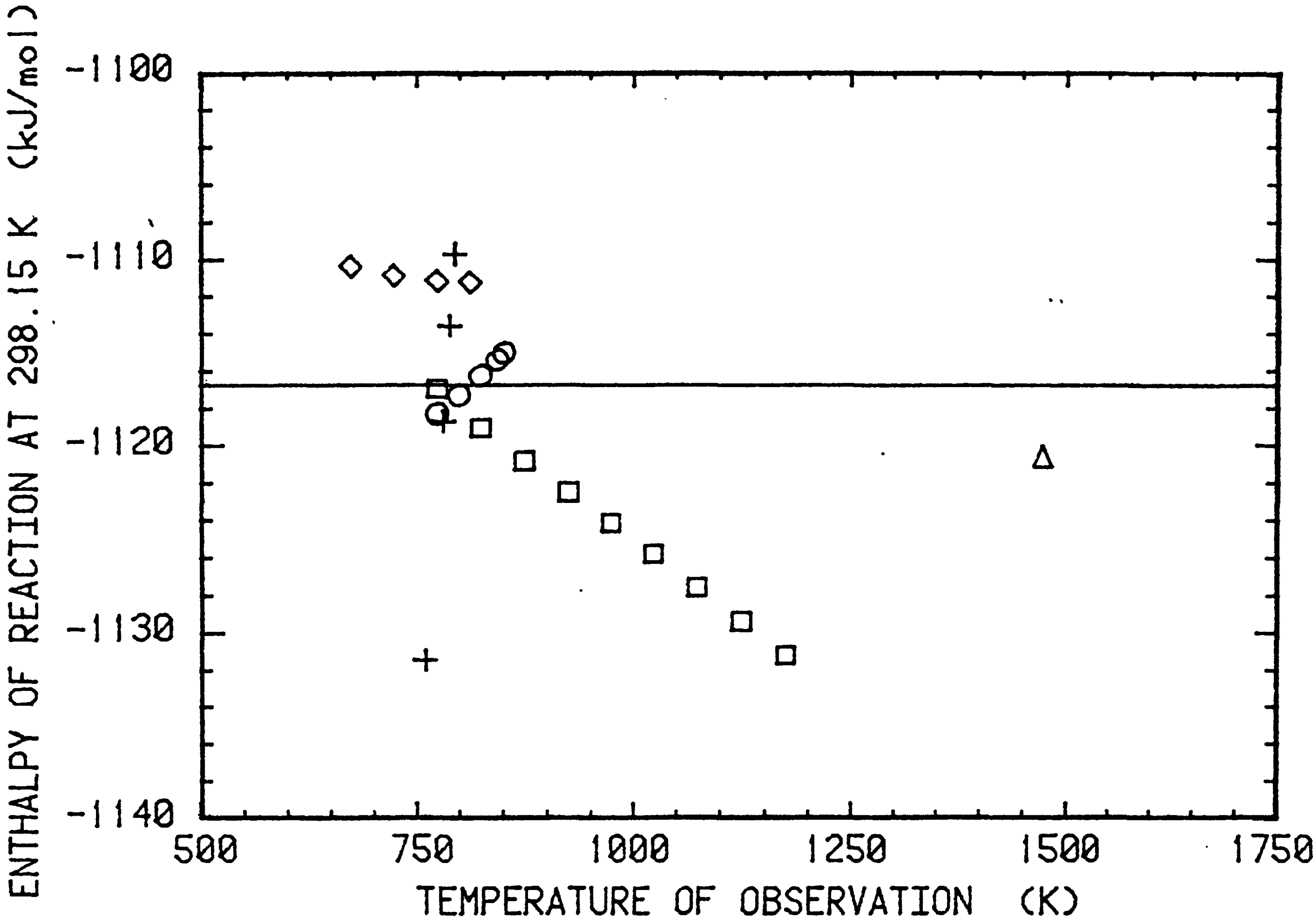
ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
-1100
-1110
-1120
-1130
-1140
500
750
1000
1250
1500
1750
TEMPERATURE OF OBSERVATION (K)

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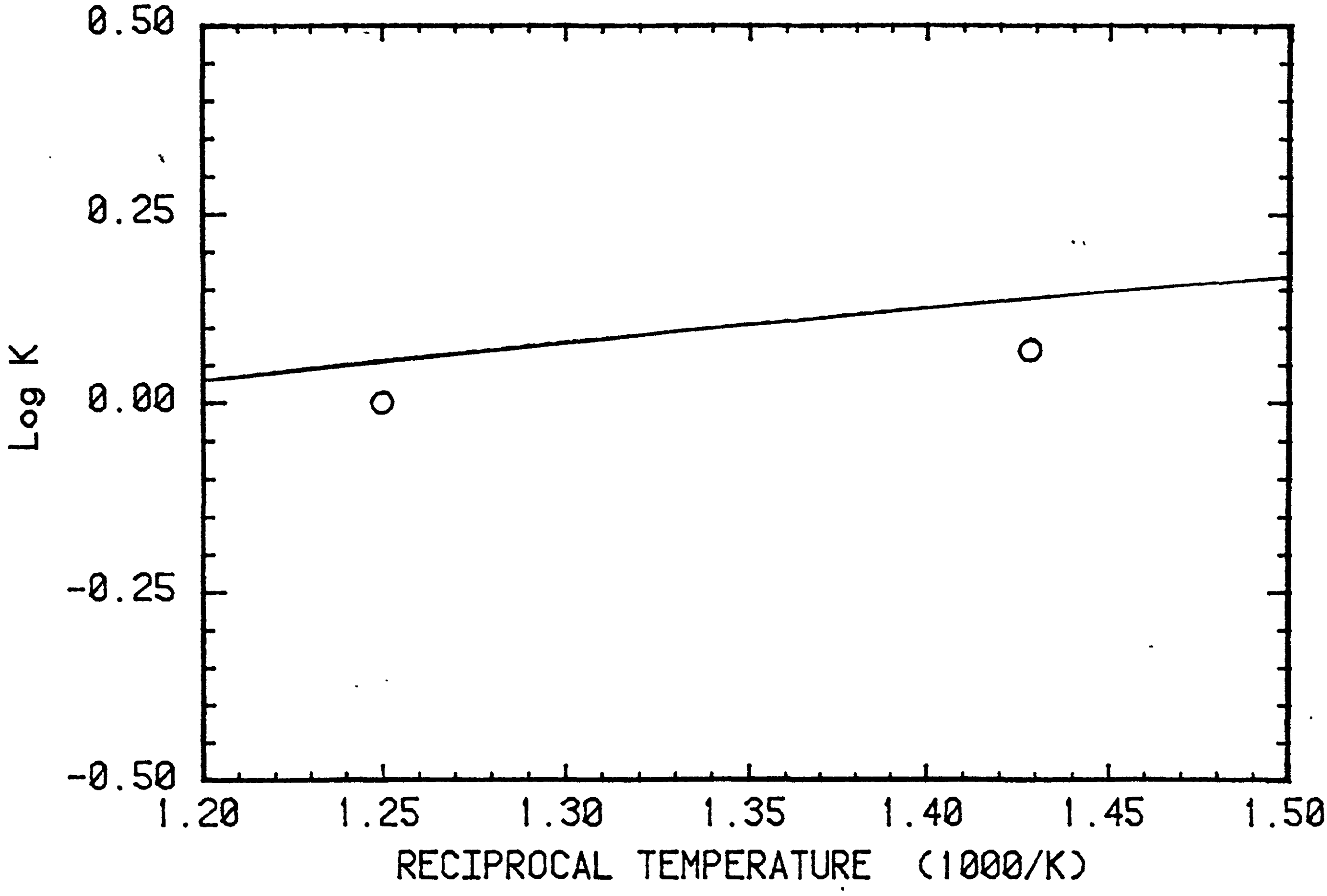
Figure A.34



548

Figure A.35

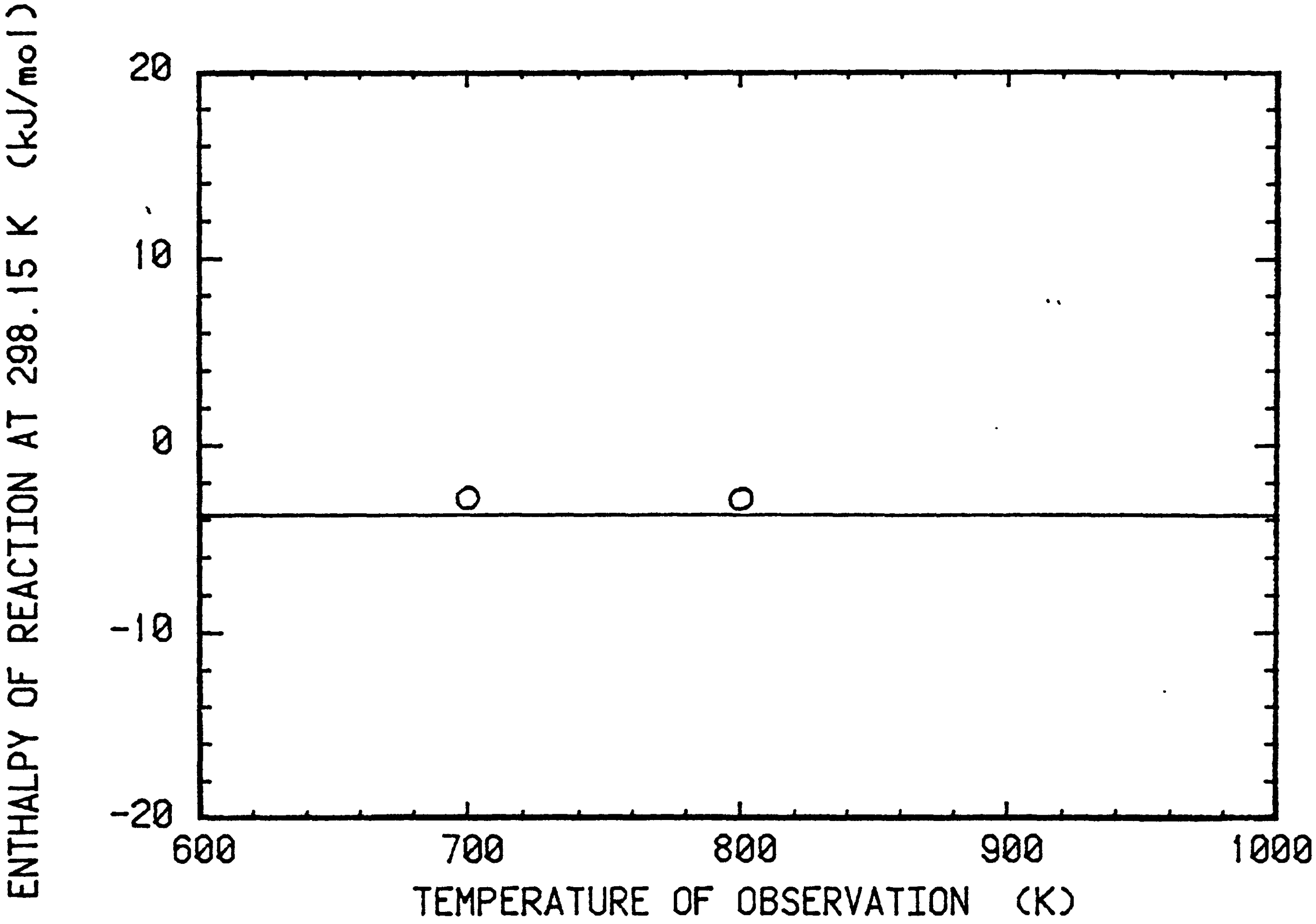

ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
20
10
0
-10
-20
600
700
800
900
1000
TEMPERATURE OF OBSERVATION (K)

Figure A.36

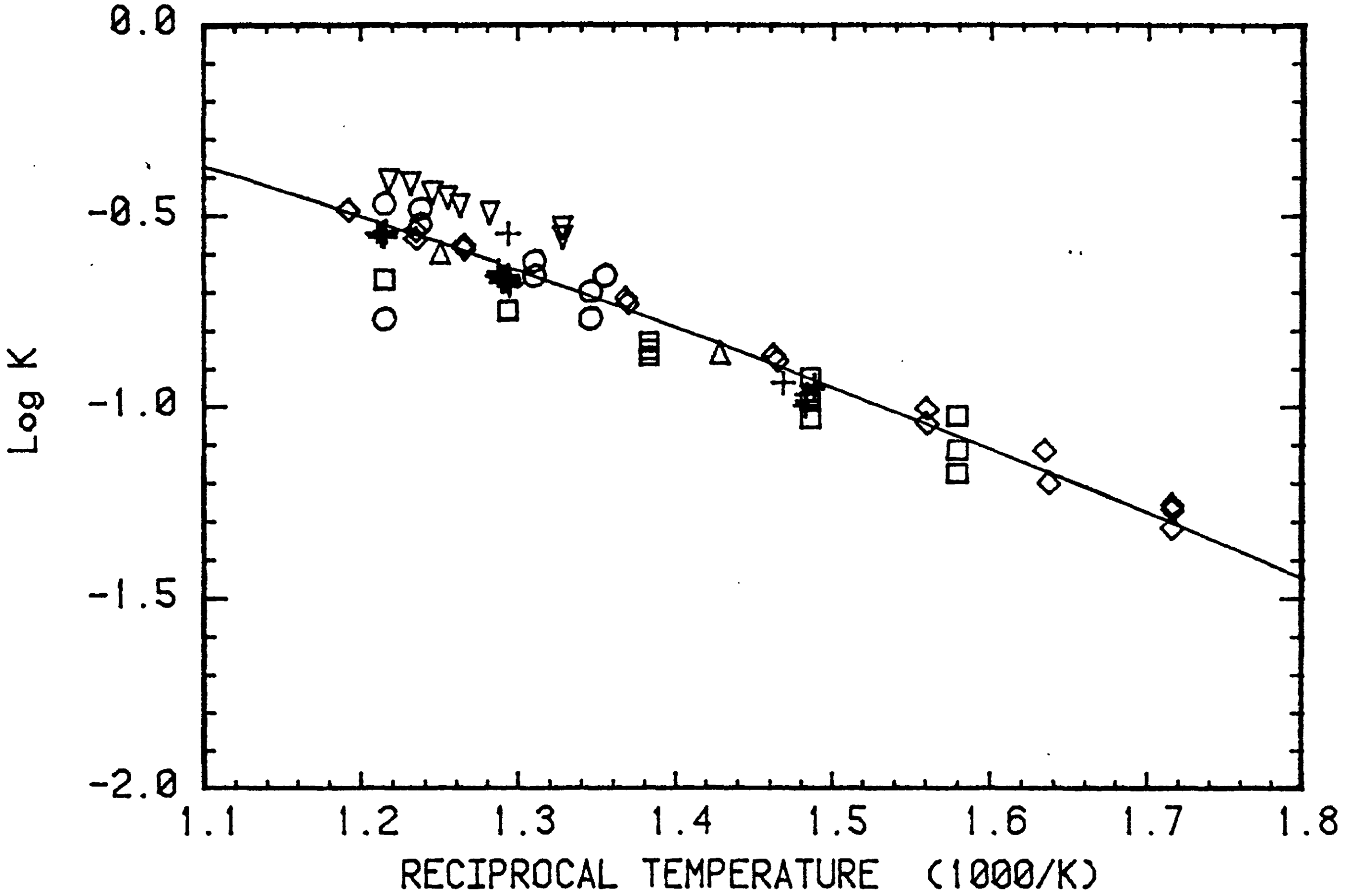

0.0
-0.5
-1.0
-1.5
-2.0
Log K
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
RECIPROCAL TEMPERATURE (1000/K)

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Figure A.37

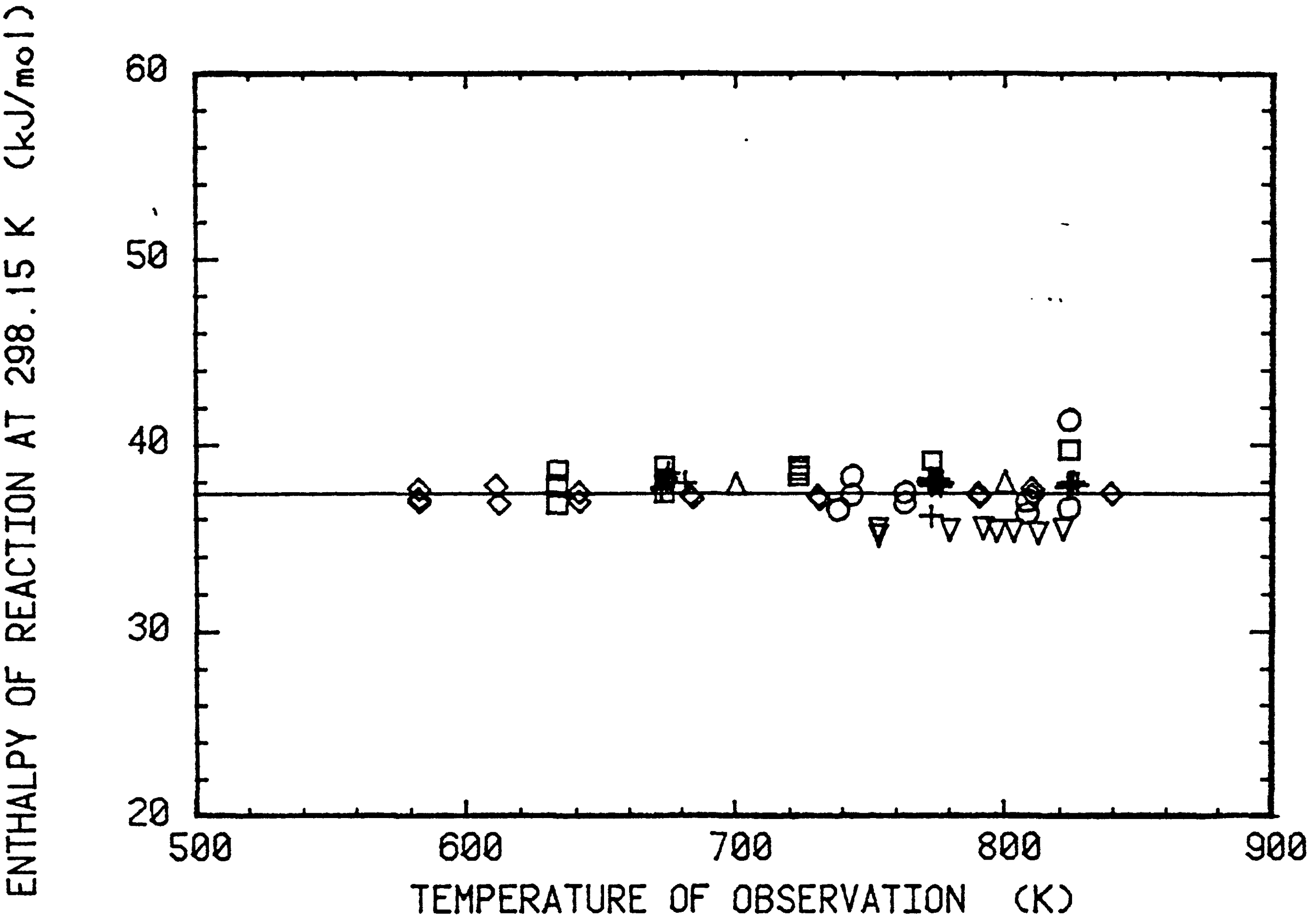


Figure A.38.

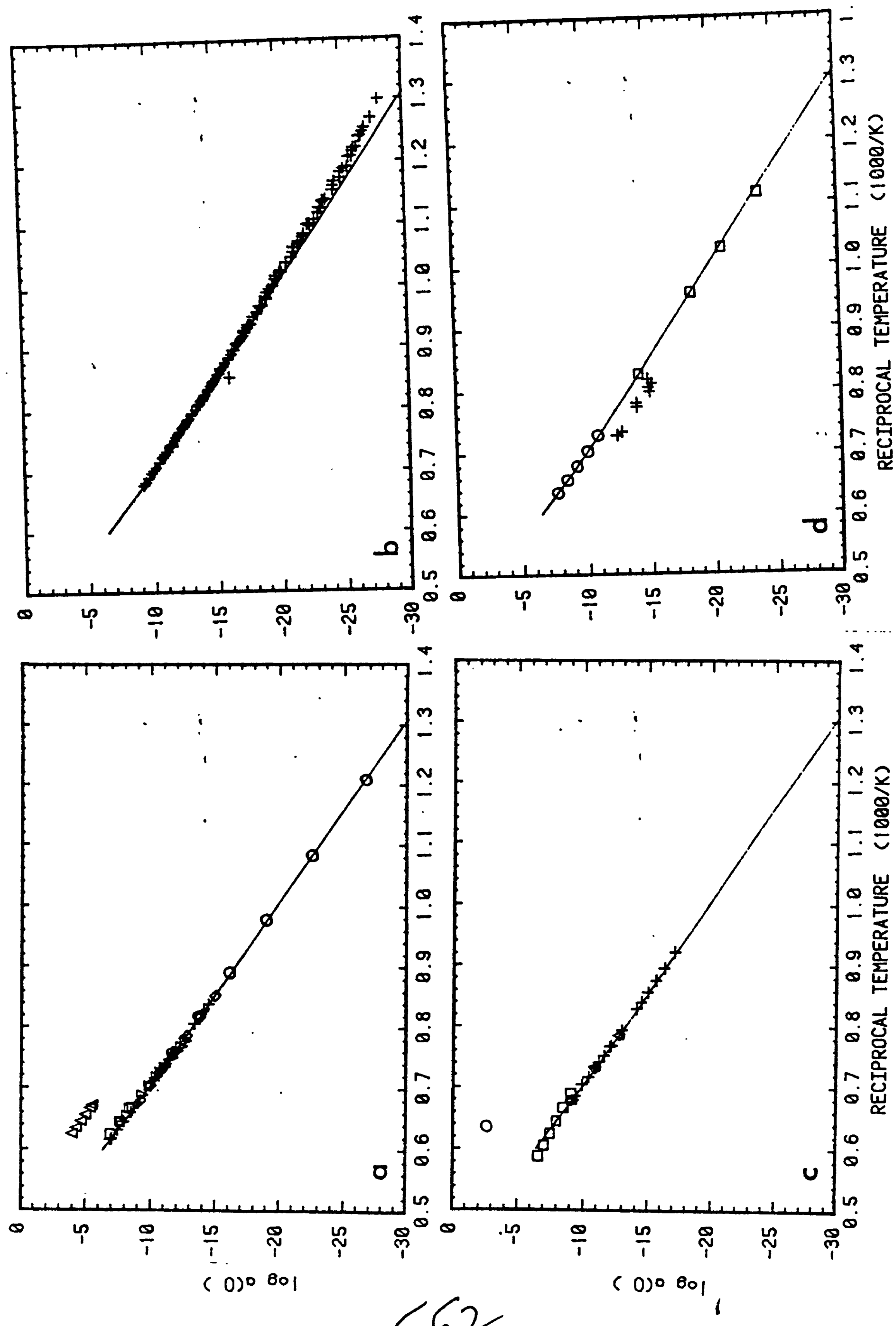

a
b
c
d
log a(O)
log a(O)
0
-5
-10
-15
-20
-25
-30
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
RECIPROCAL TEMPERATURE (1000/K)
RECIPROCAL TEMPERATURE (1000/K)

Figure A.39.

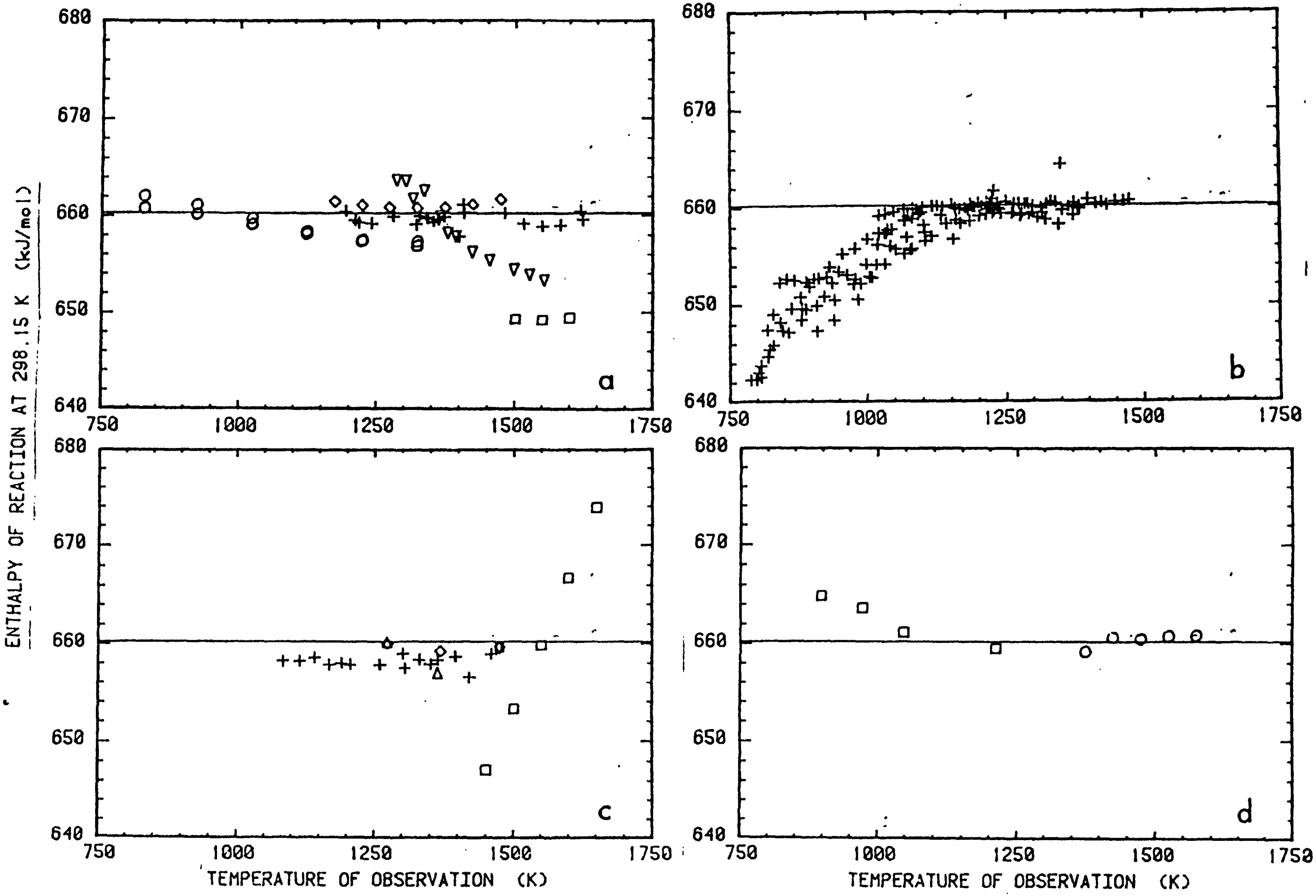
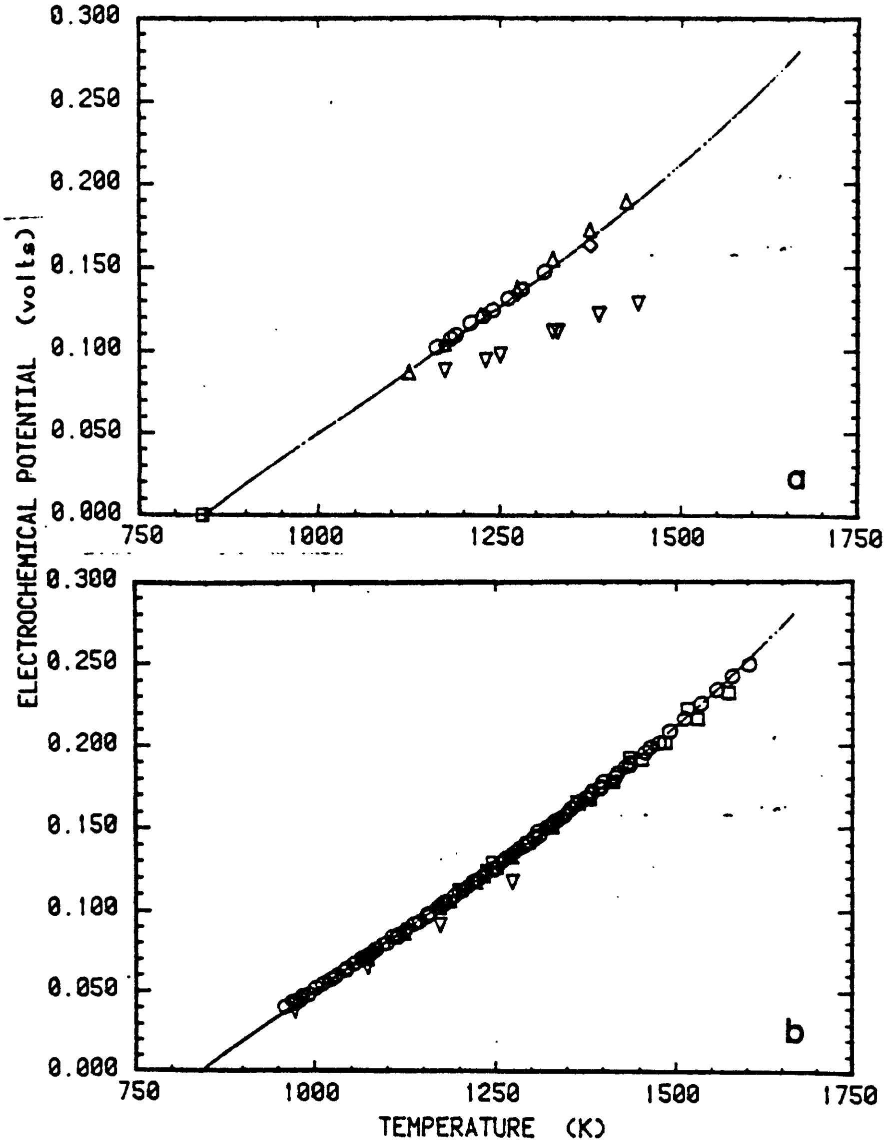

a
b
c
d
680
670
660
650
640
750
1000
1250
1500
1750
ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
TEMPERATURE OF OBSERVATION (K)

Figure A.40.



554

Figure A.41.

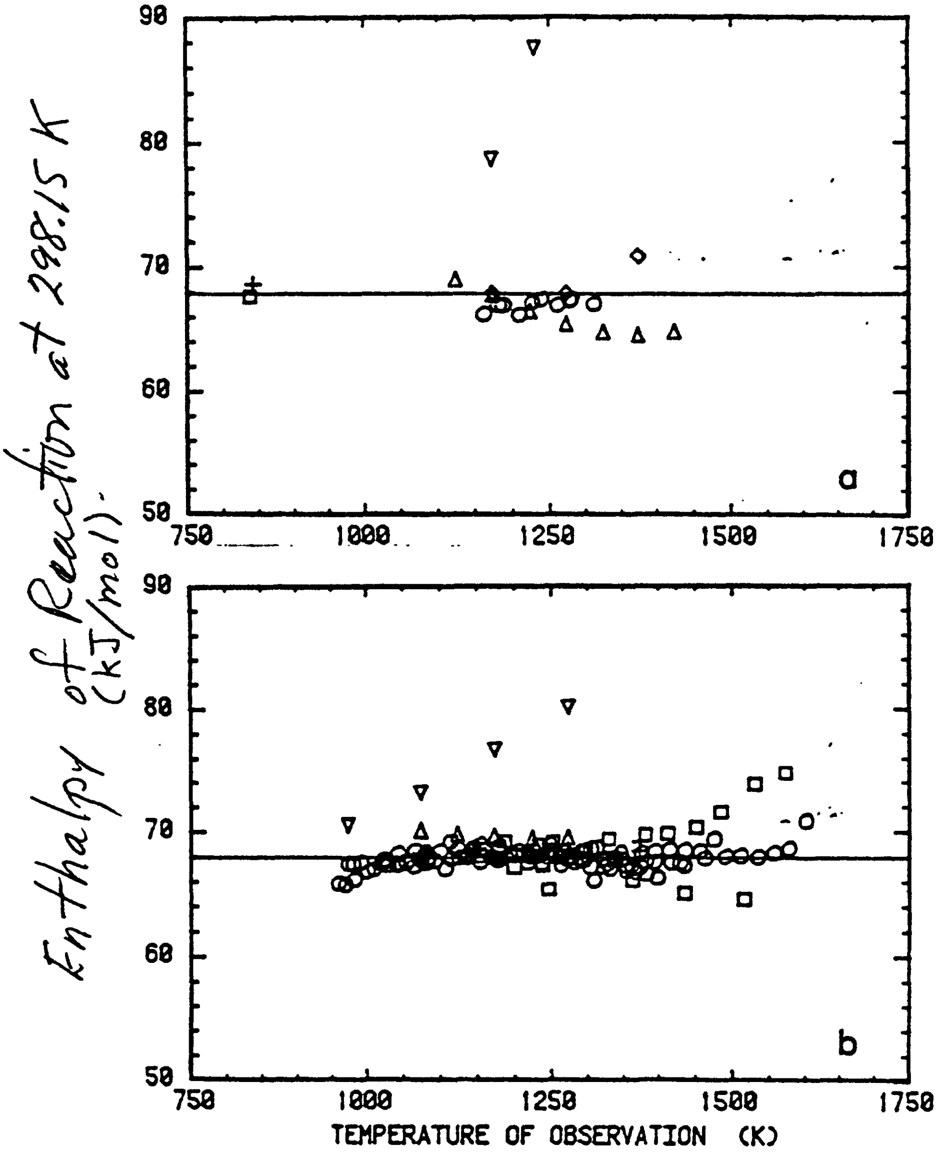

Enthalpy of Reaction at 298.15 K (kJ/mol).
90
80
70
60
50
a
750
1000
1250
1500
1750
90
80
70
60
50
b
750
1000
1250
1500
1750
TEMPERATURE OF OBSERVATION (K)

Figure A.42.

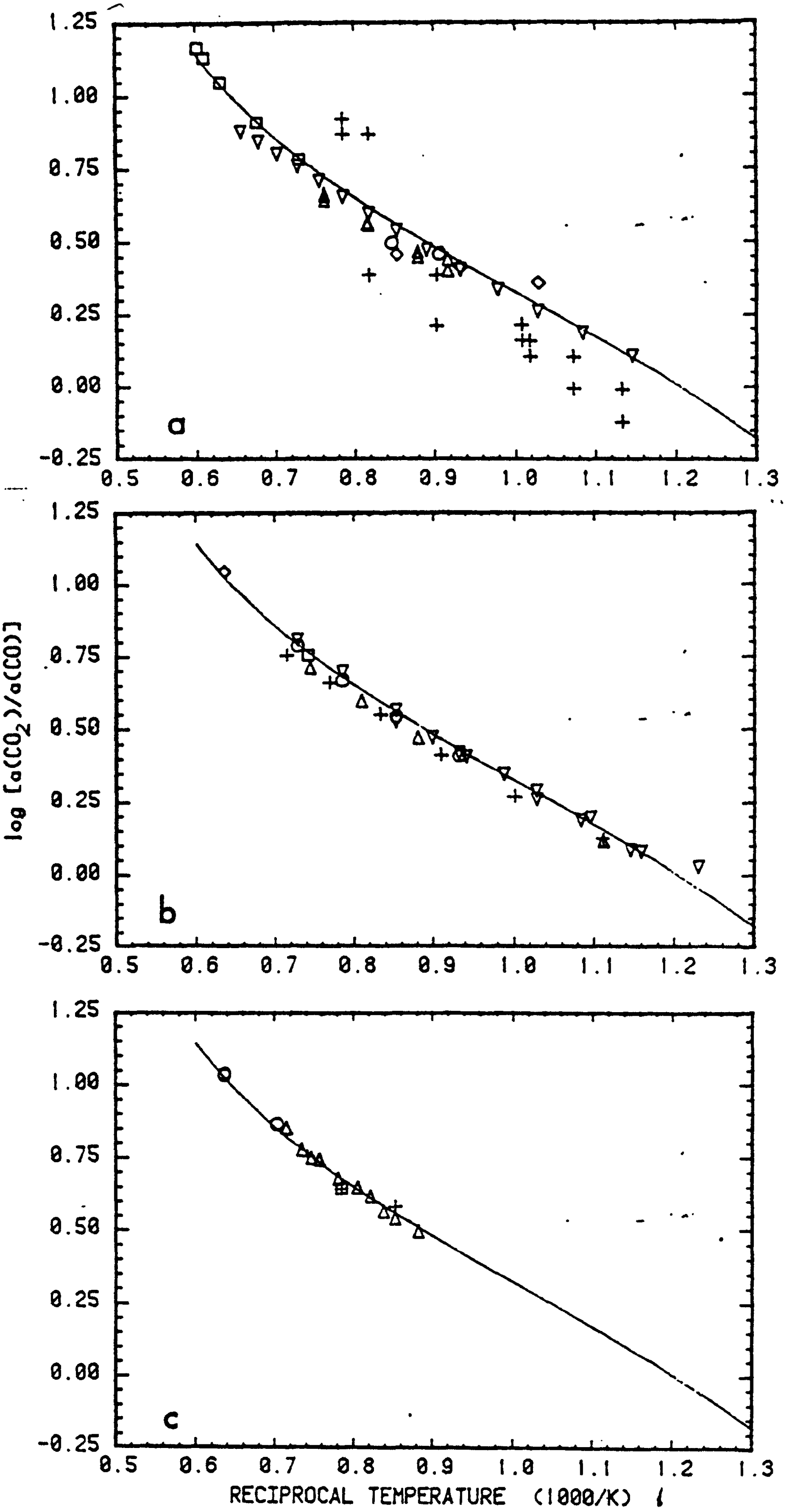

1.25
1.00
0.75
0.50
0.25
0.00
-0.25
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
a
b
c
log [a(CO$_2$)/a(CO)]
RECIPROCAL TEMPERATURE (1000/K)

Figure A.43.

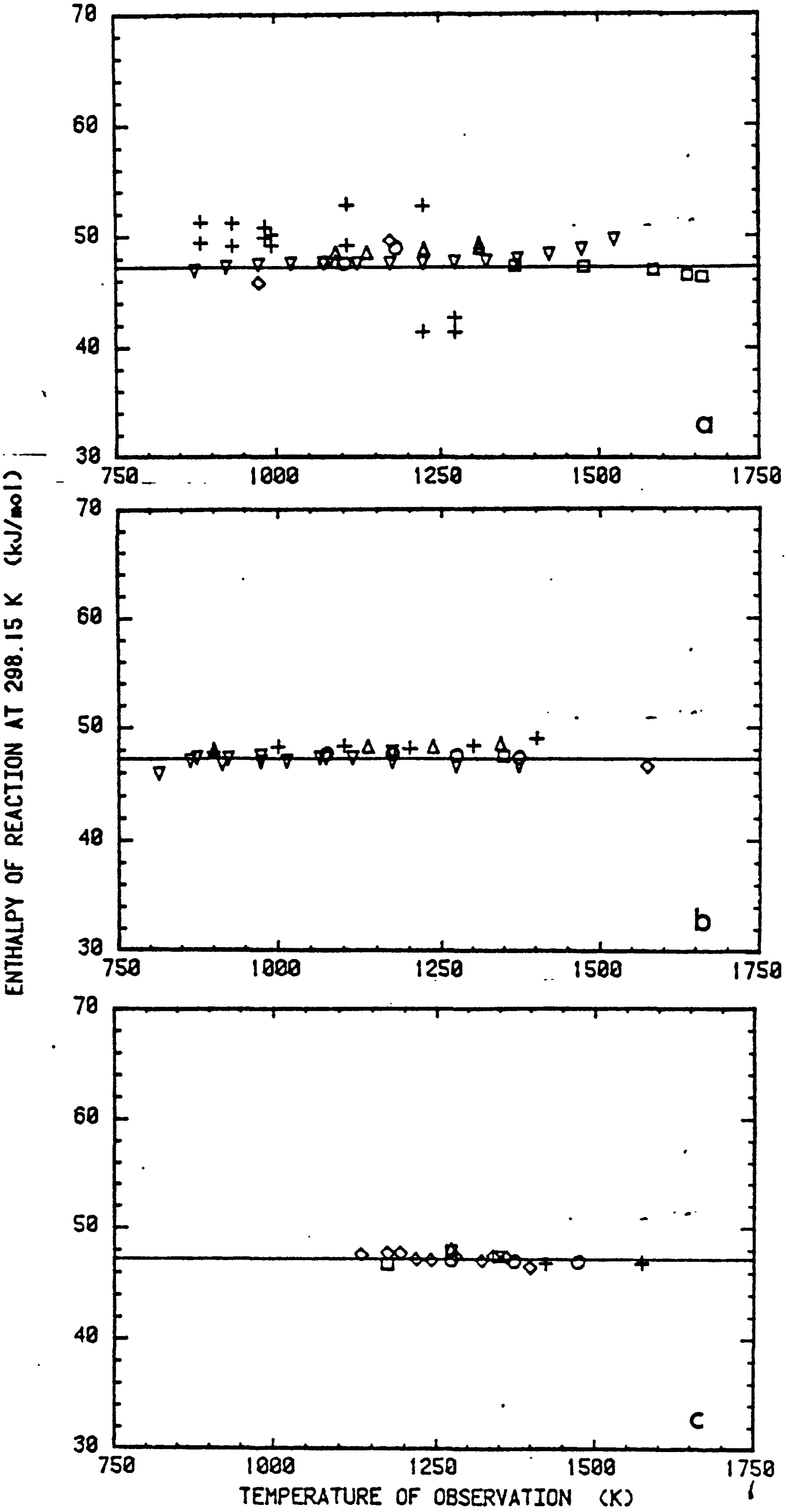

70
60
50
40
30
750
1000
1250
1500
1750
a
b
c
ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
TEMPERATURE OF OBSERVATION (K)

Figure A.44.

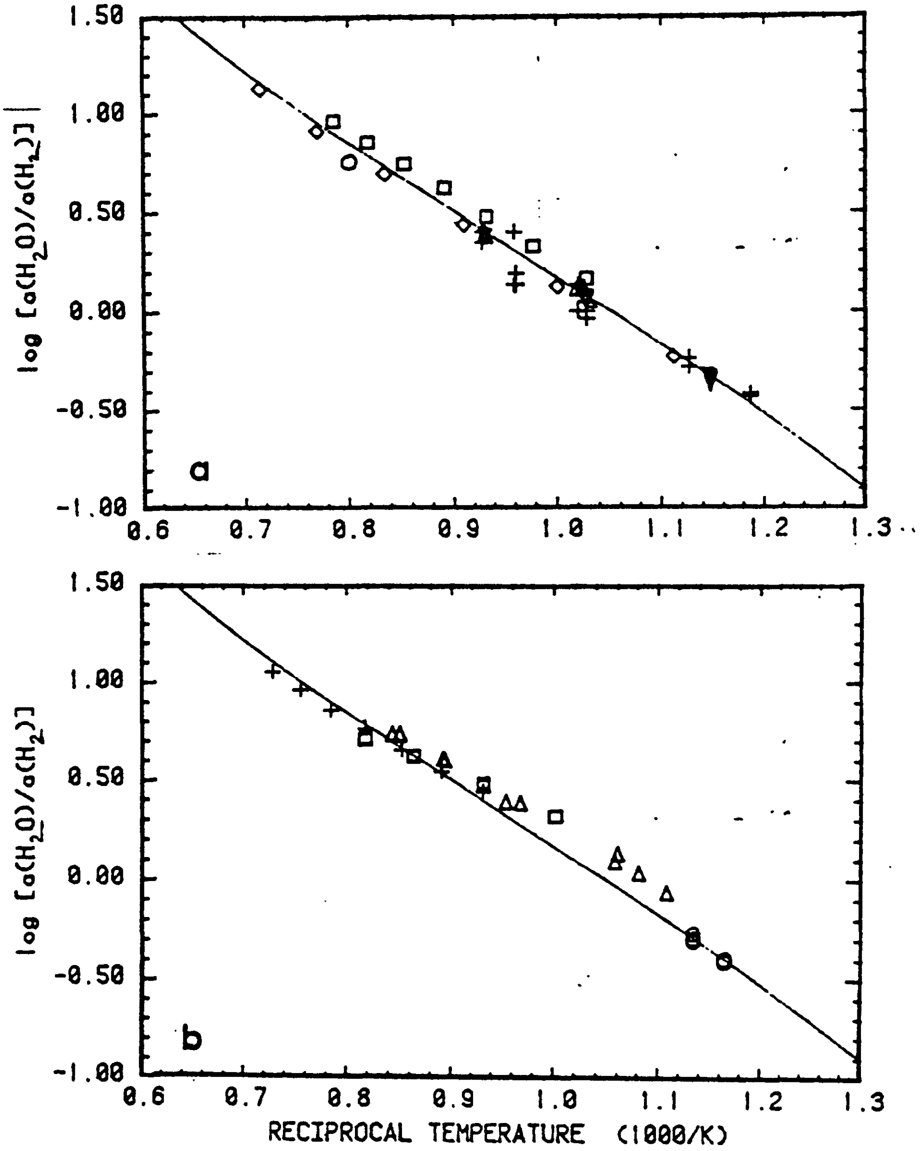

1.50
1.00
0.50
0.00
-0.50
-1.00
log [$a(H_2O)/a(H_2)$]
a
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
b
RECIPROCAL TEMPERATURE (1000/K)

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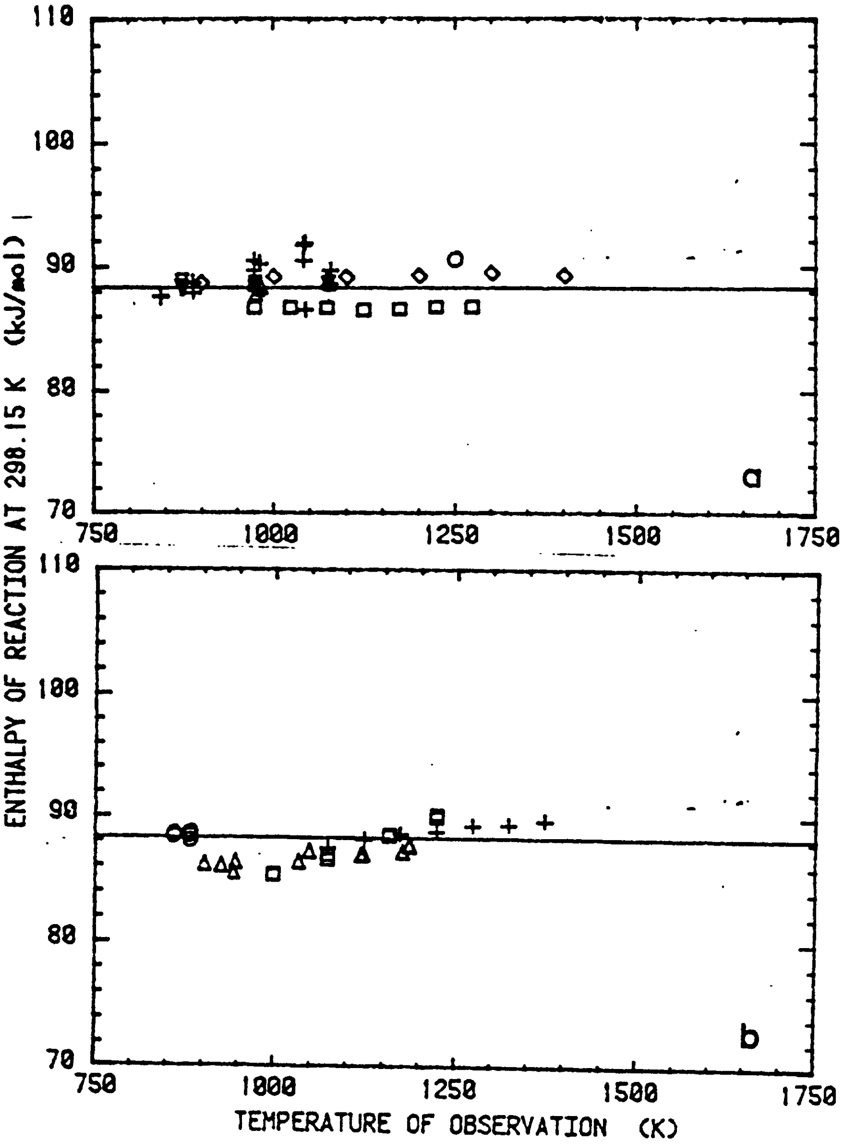
Figure A.45.



559

Figure A.46

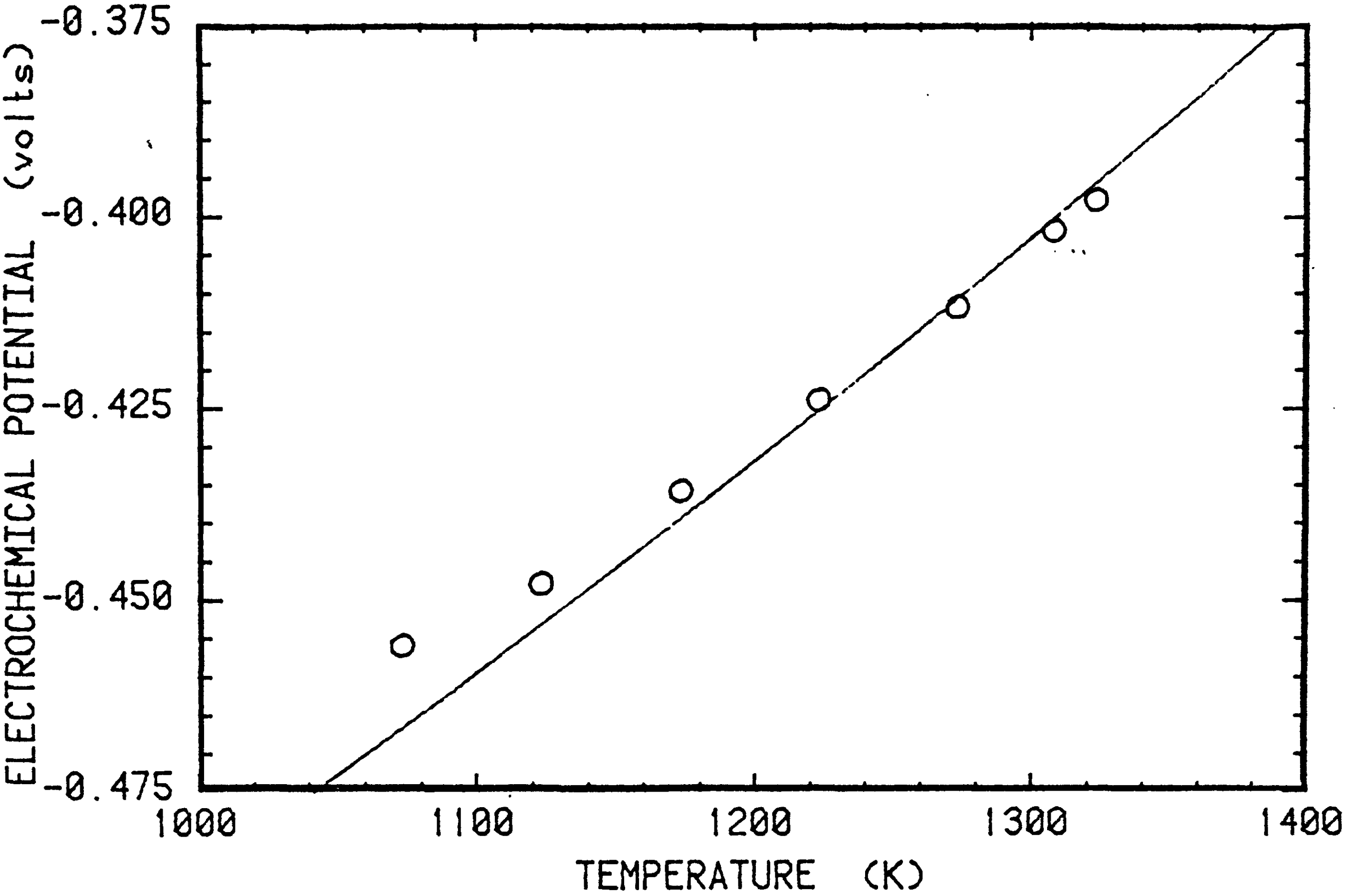

-0.375
-0.400
-0.425
-0.450
-0.475
ELECTROCHEMICAL POTENTIAL (volts)
1000
1100
1200
1300
1400
TEMPERATURE (K)

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Figure A.47

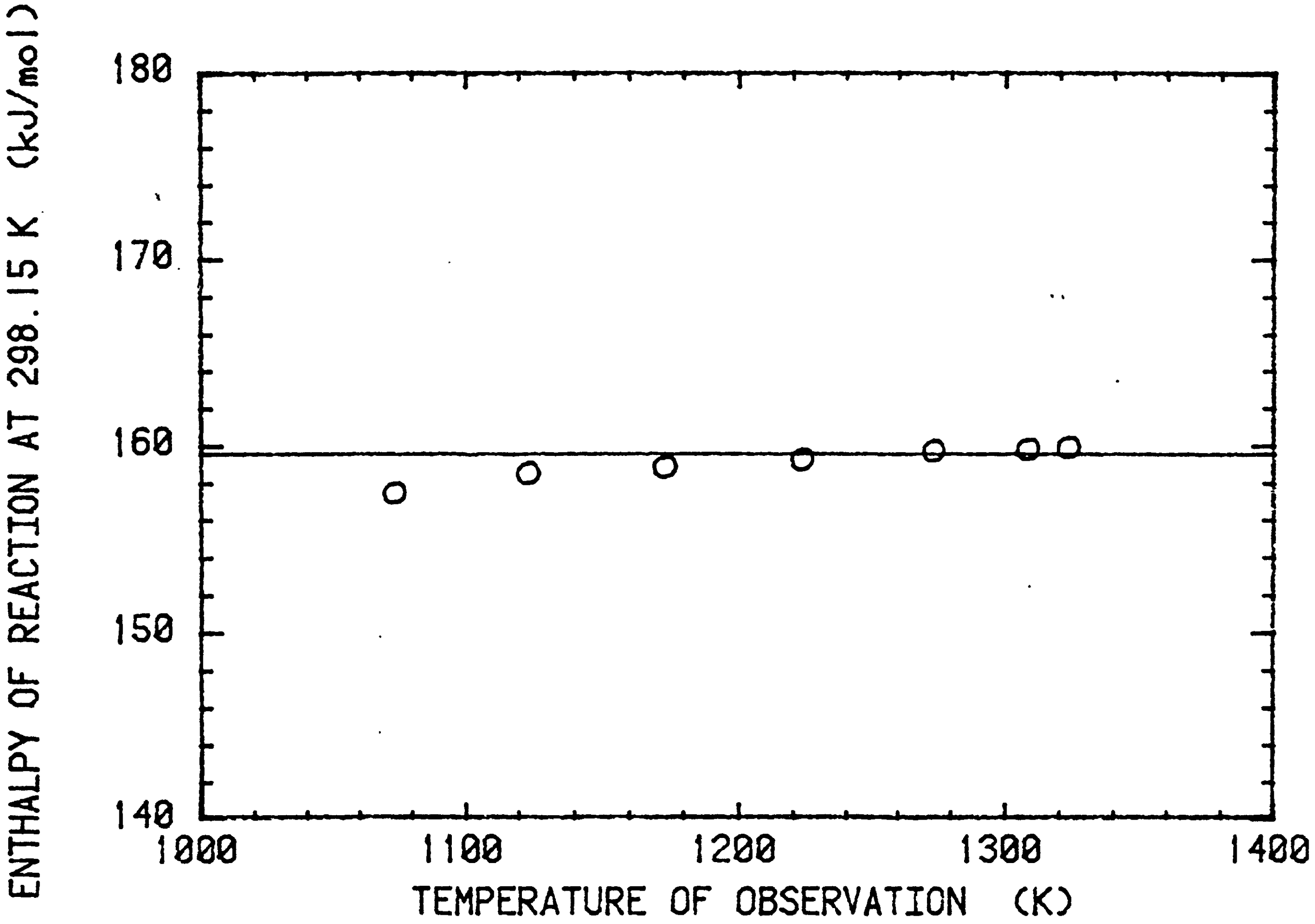

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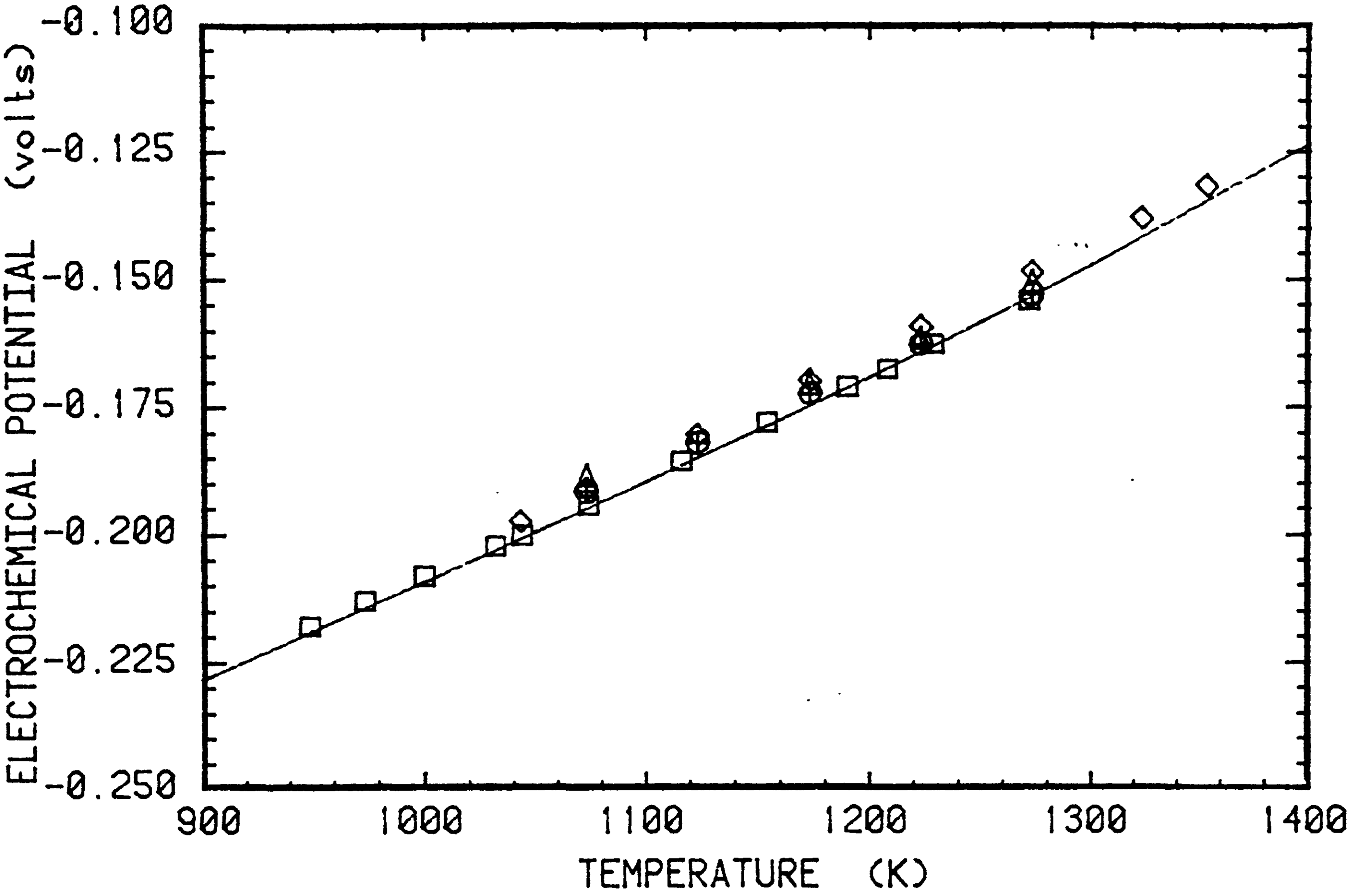
Figure A.48



562

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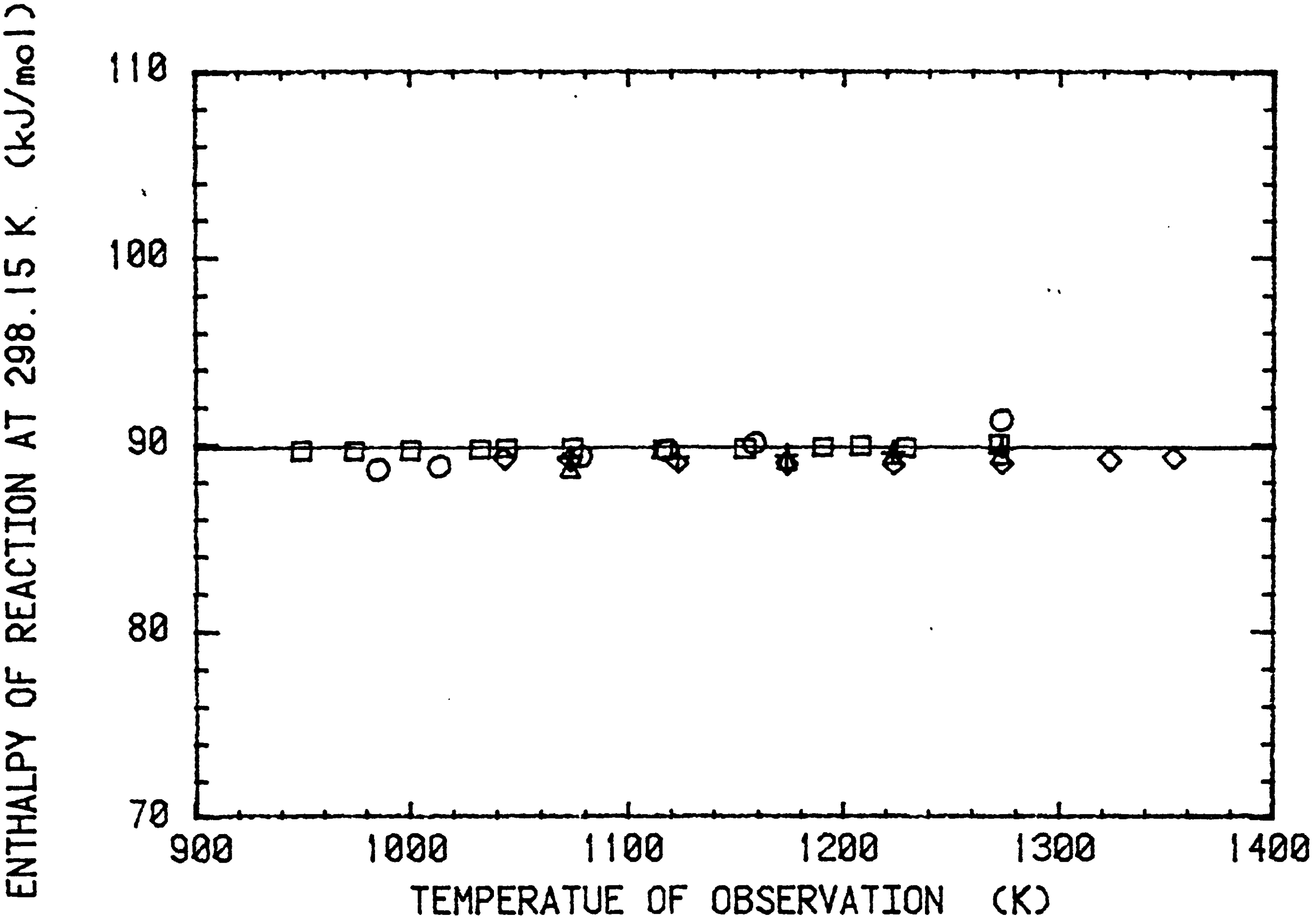
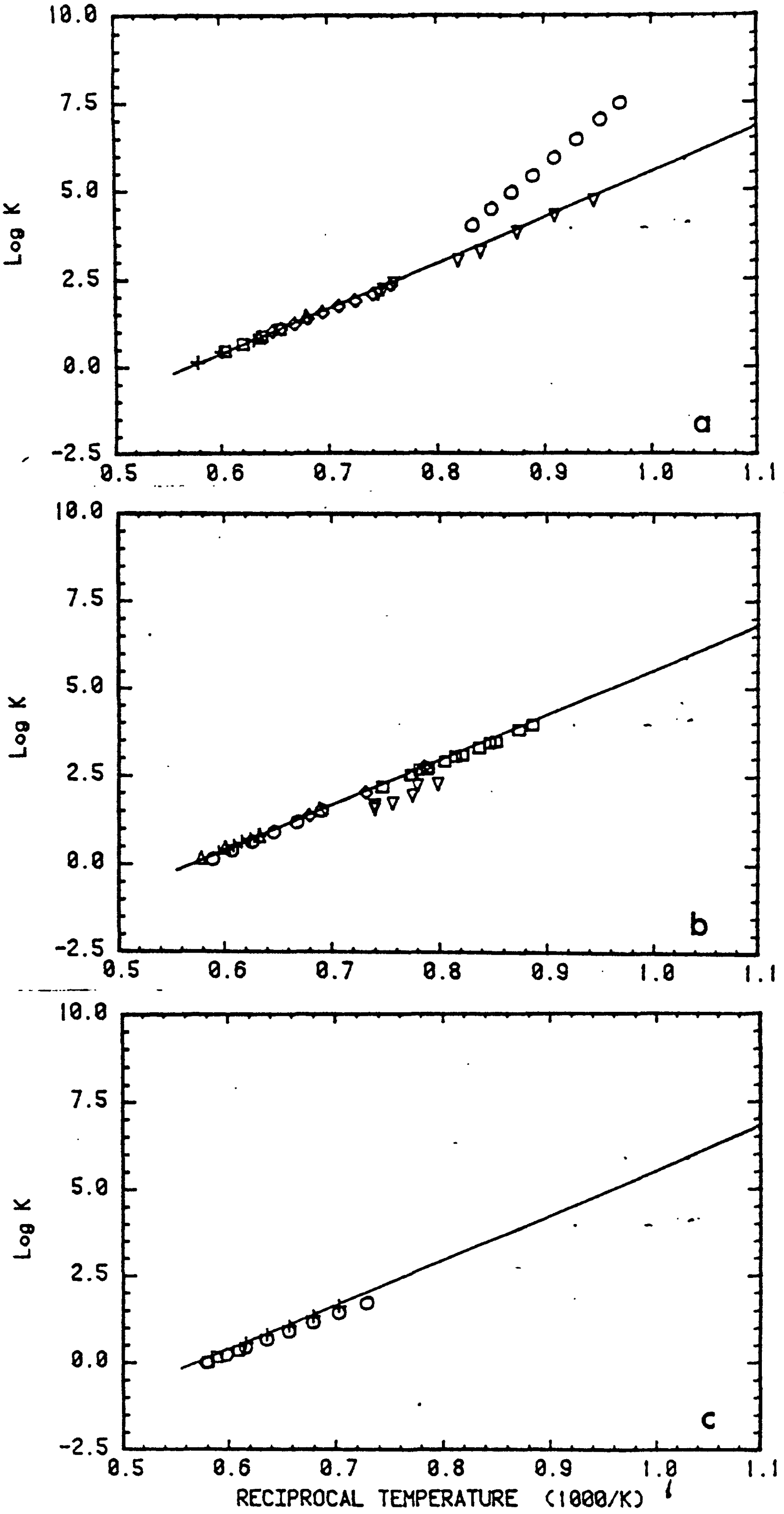
Figure A.49



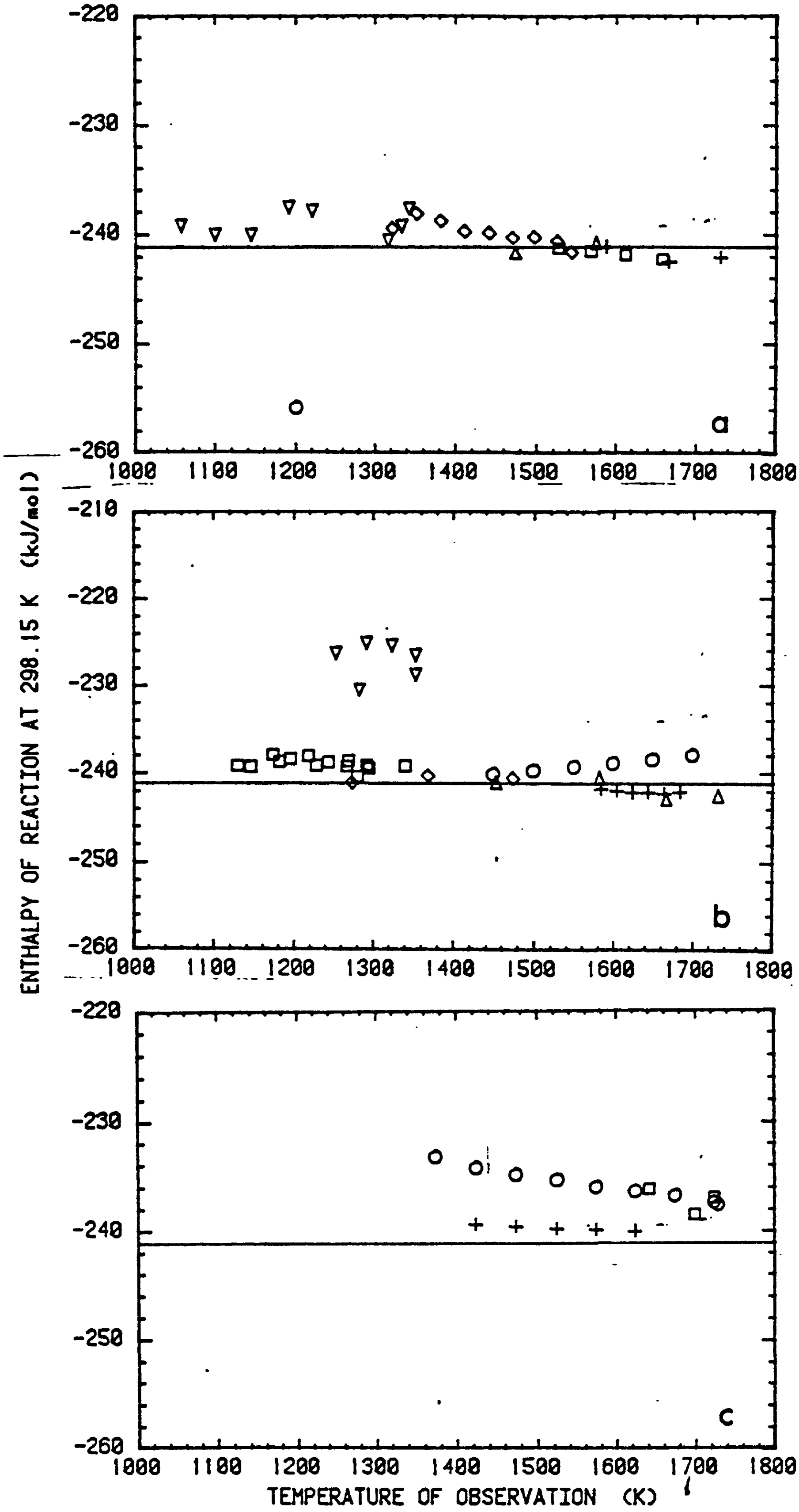
563

Figure A.50.



564

Figure A.51,



565

Figure A.52

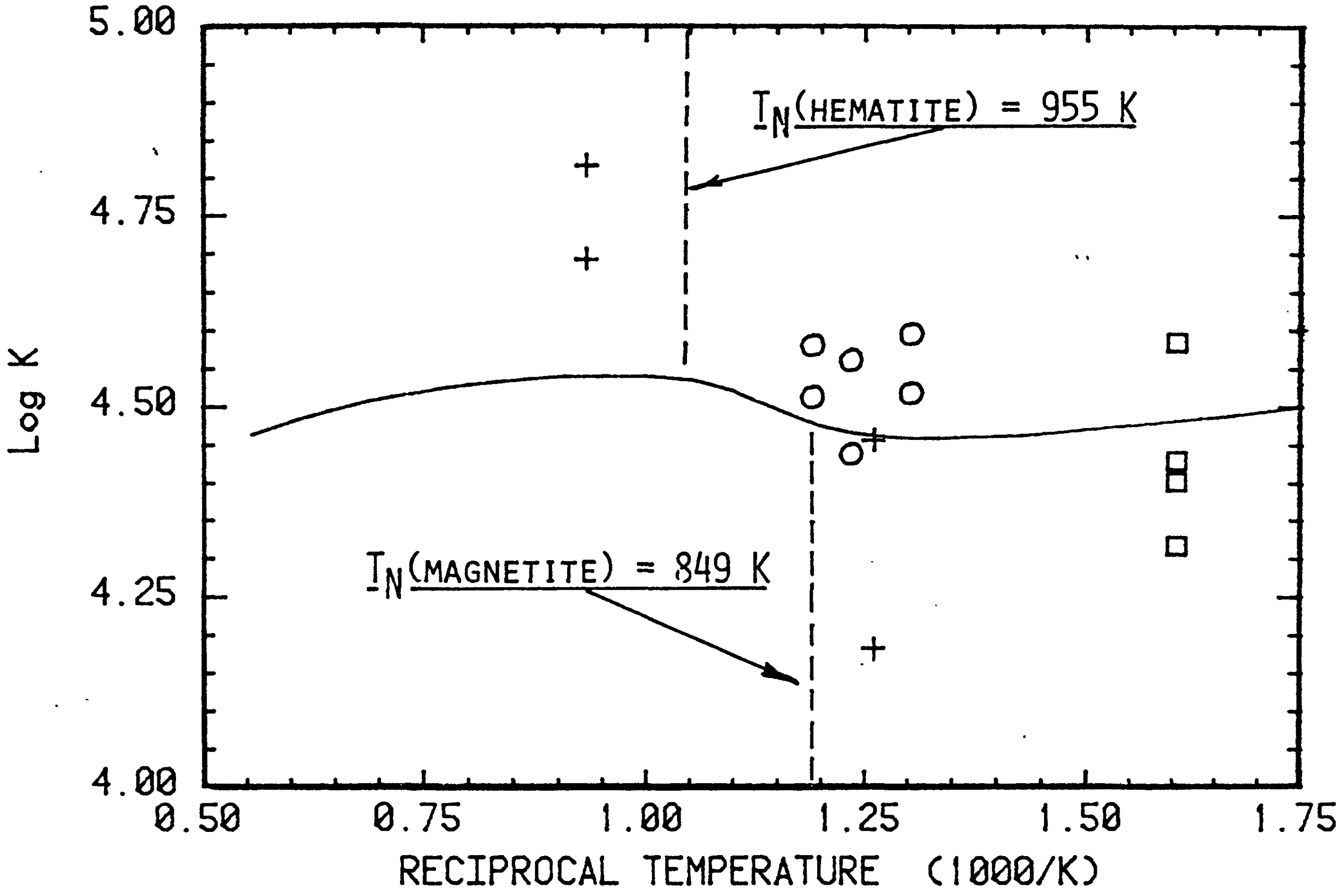

5.00
4.75
4.50
4.25
4.00
Log K
0.50
0.75
1.00
1.25
1.50
1.75
RECIPROCAL TEMPERATURE (1000/K)
T_N(HEMATITE) = 955 K
T_N(MAGNETITE) = 849 K

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Figure A.53

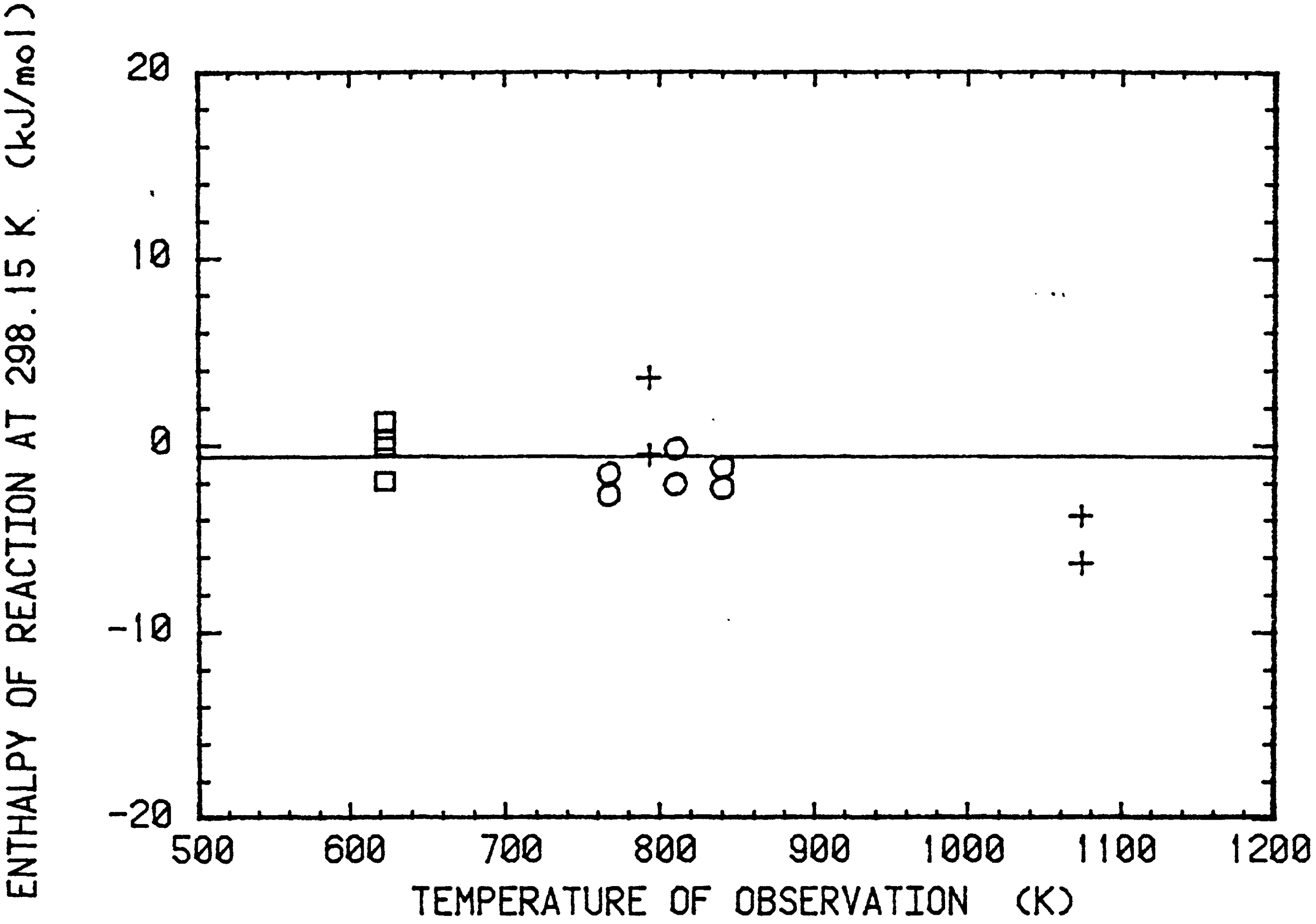


Figure A.54

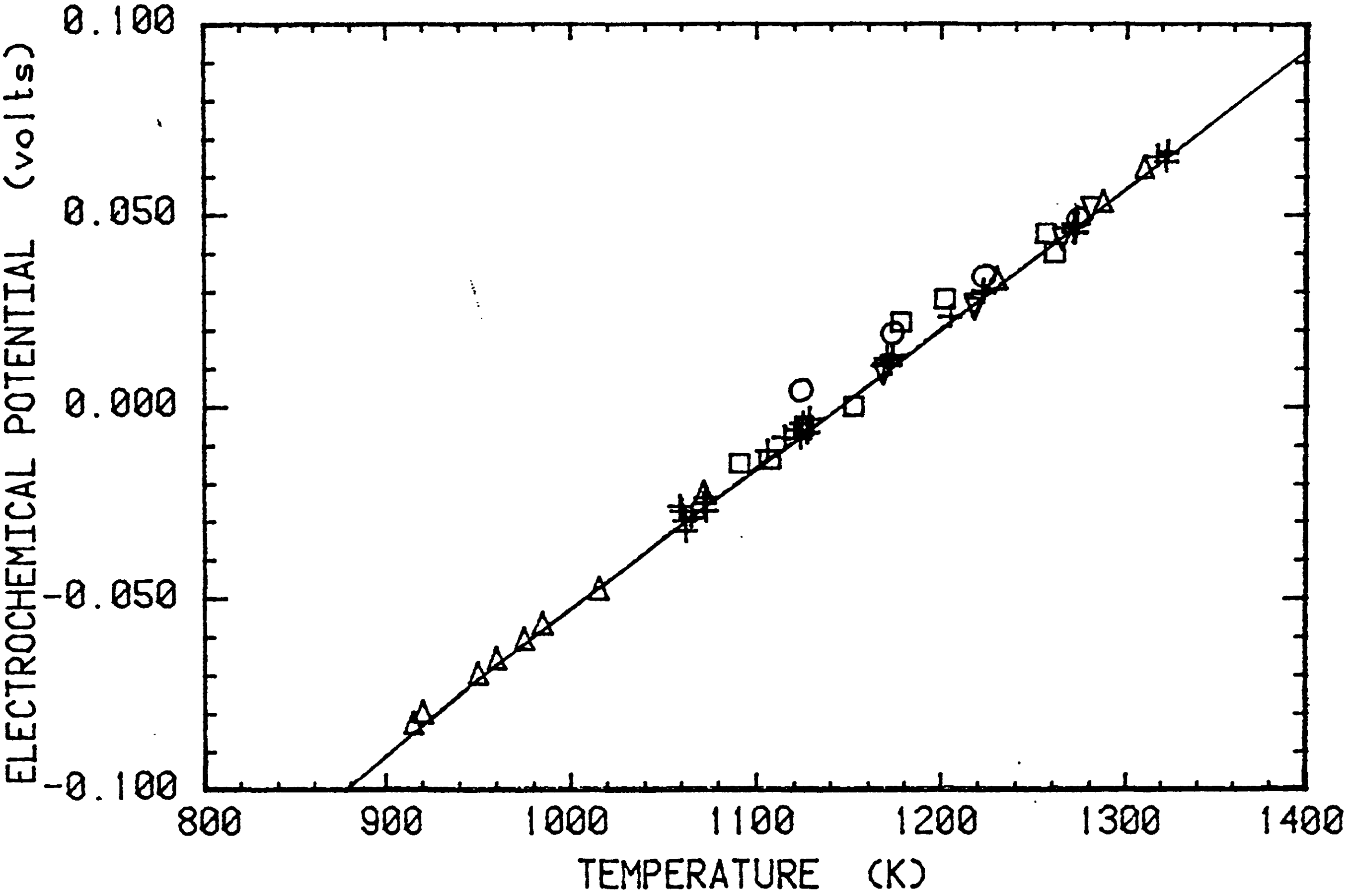
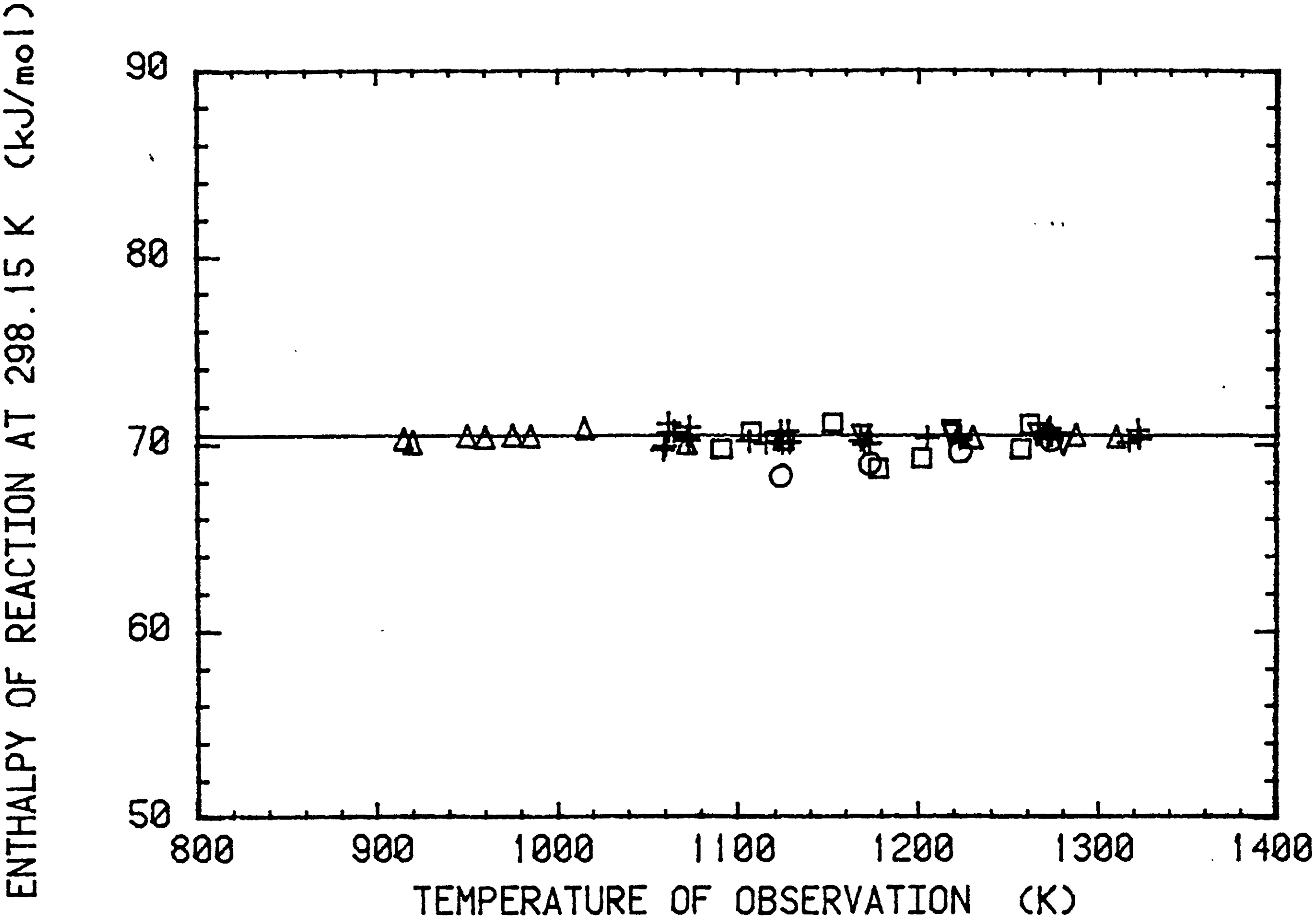

0.100
0.050
0.000
-0.050
-0.100
ELECTROCHEMICAL POTENTIAL (volts)
800
900
1000
1100
1200
1300
1400
TEMPERATURE (K)

Figure A.55


ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
90
80
70
60
50
800
900
1000
1100
1200
1300
1400
TEMPERATURE OF OBSERVATION (K)

J.L. Haas, Jr., "Oxygen Buffers" 1-Dec-87

Figure A.56

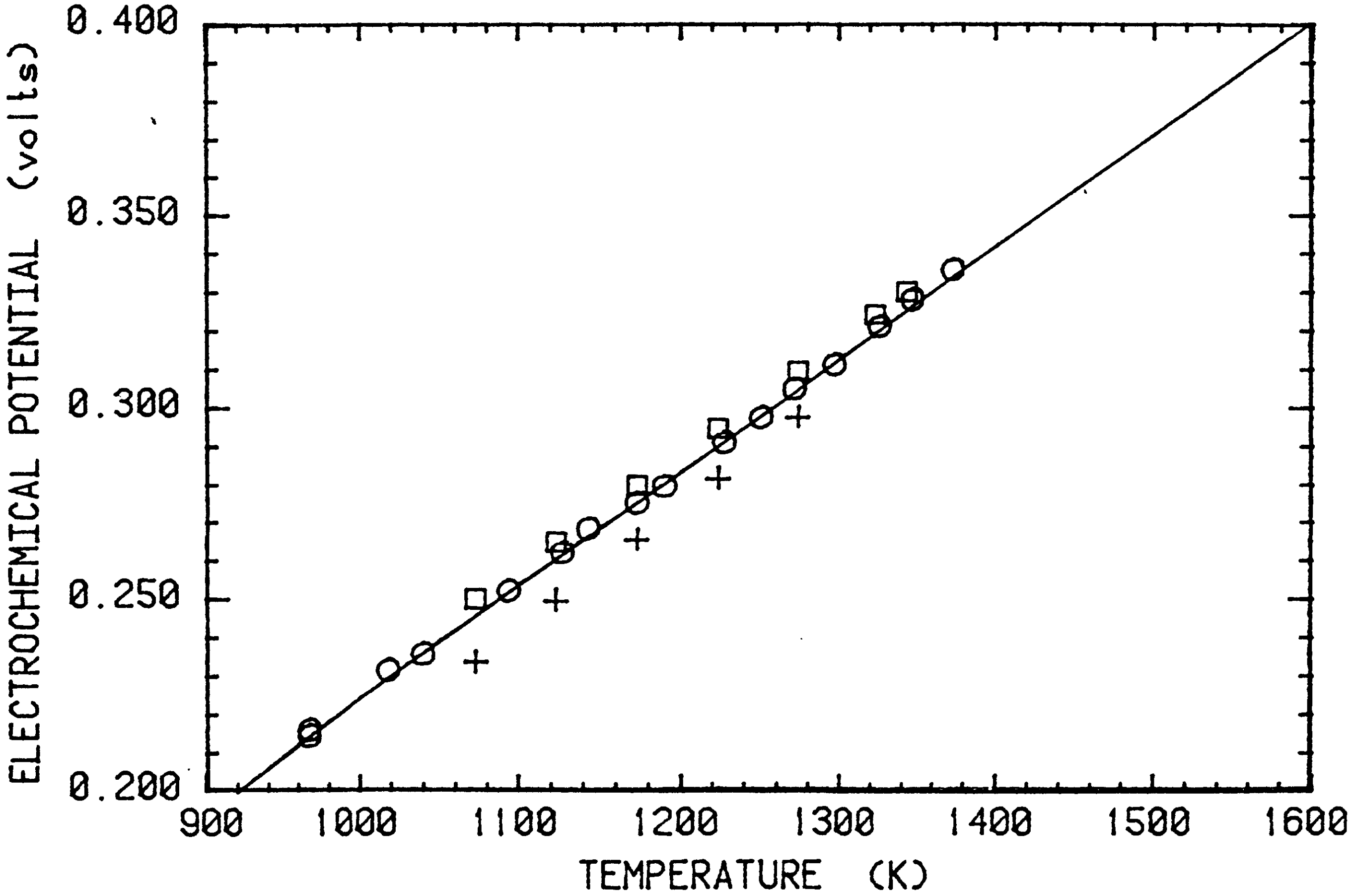


Figure A.57

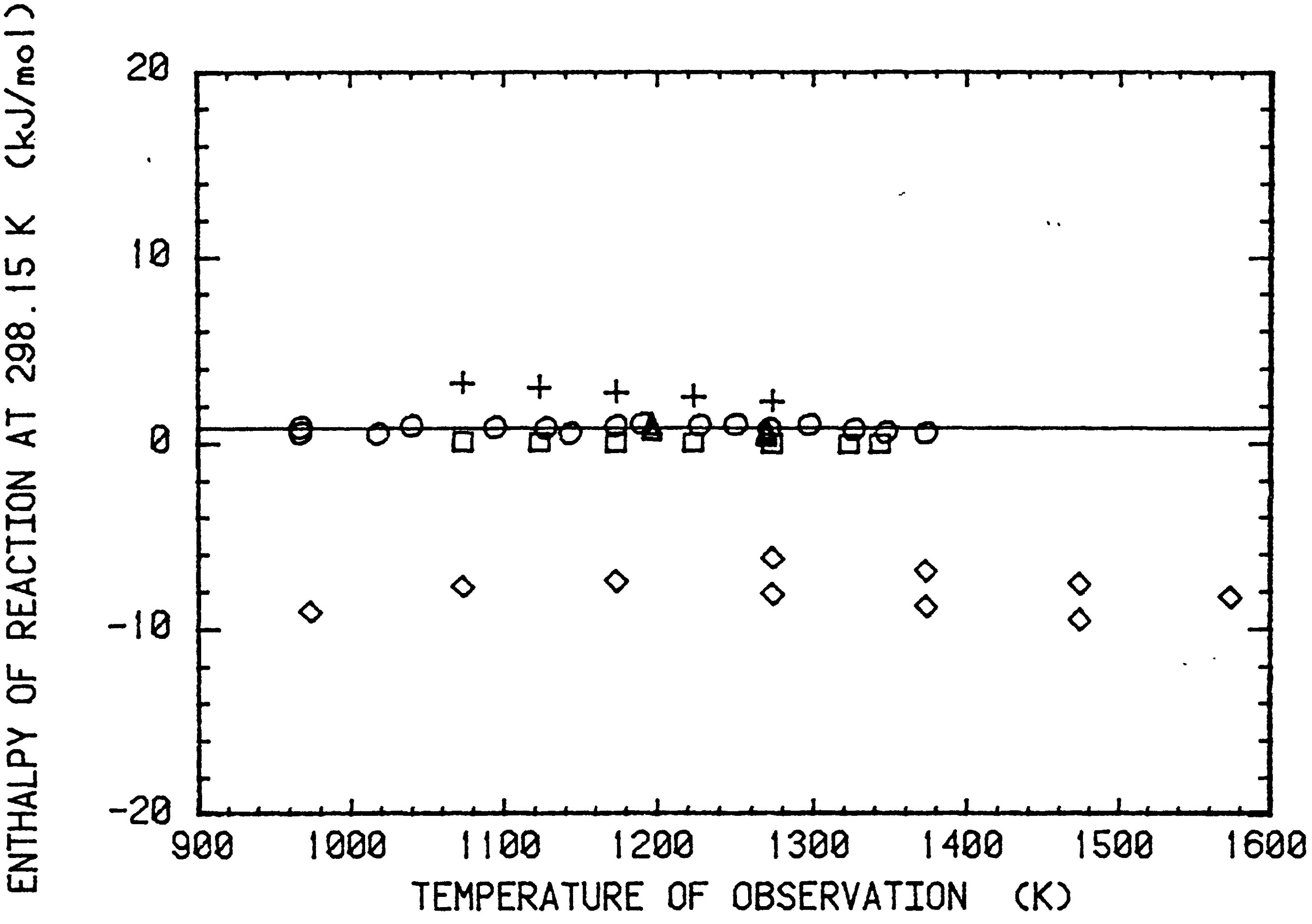
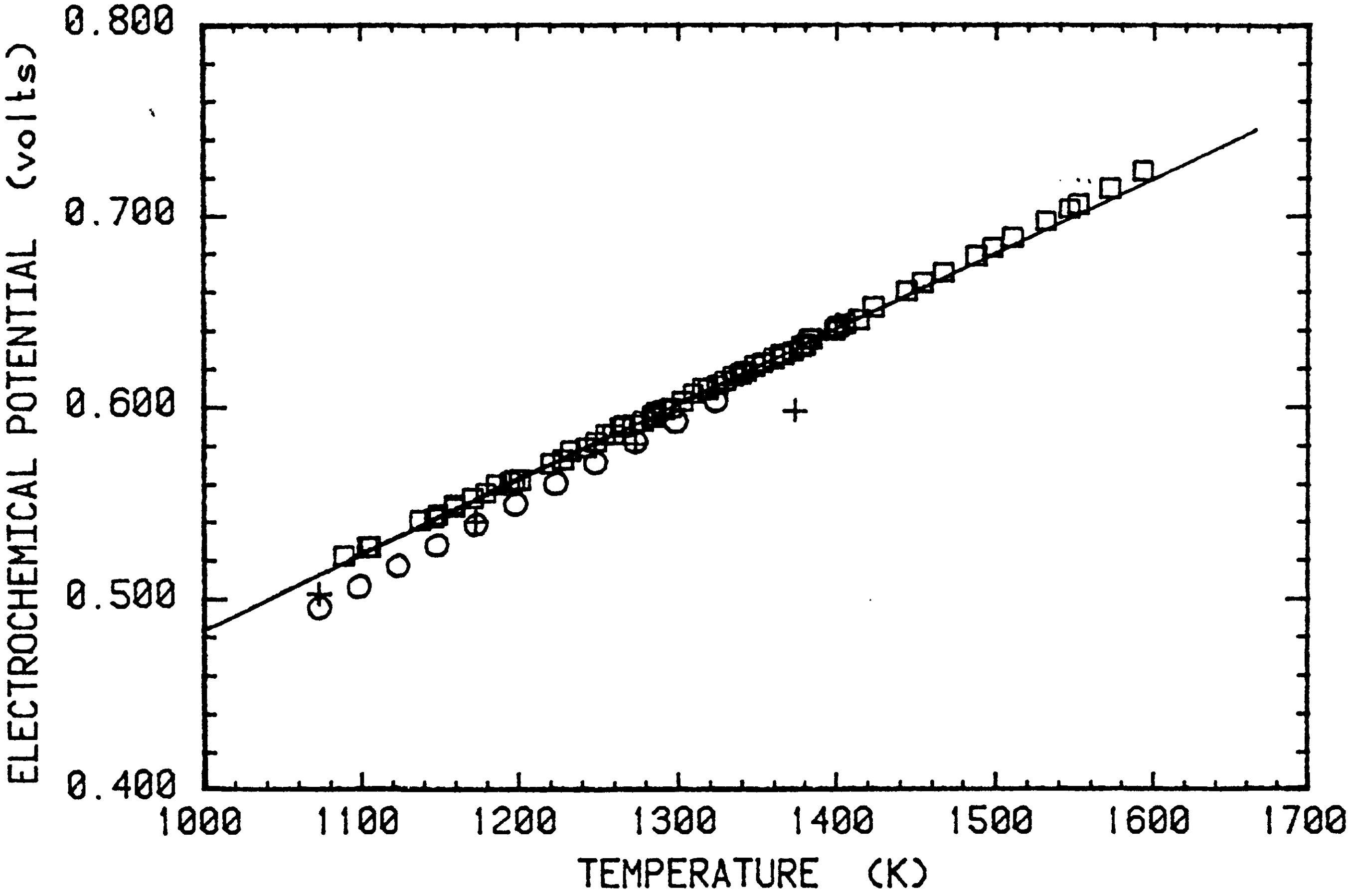

ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
20
10
0
-10
-20
900
1000
1100
1200
1300
1400
1500
1600
TEMPERATURE OF OBSERVATION (K)

Figure A.58



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J.L. Haas, Jr., "Oxygen Buffers" 1 Dec 87

Figure A.59

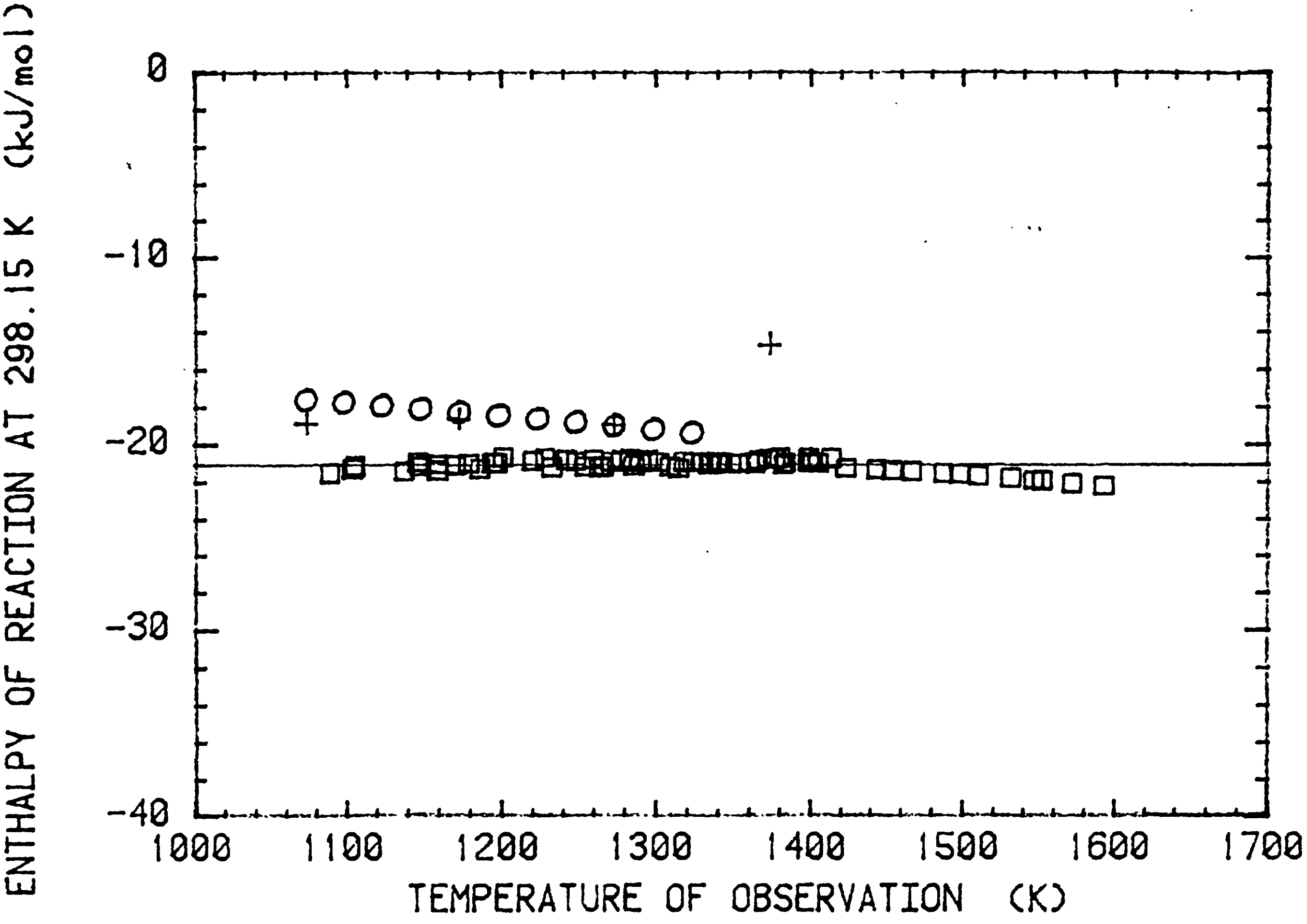
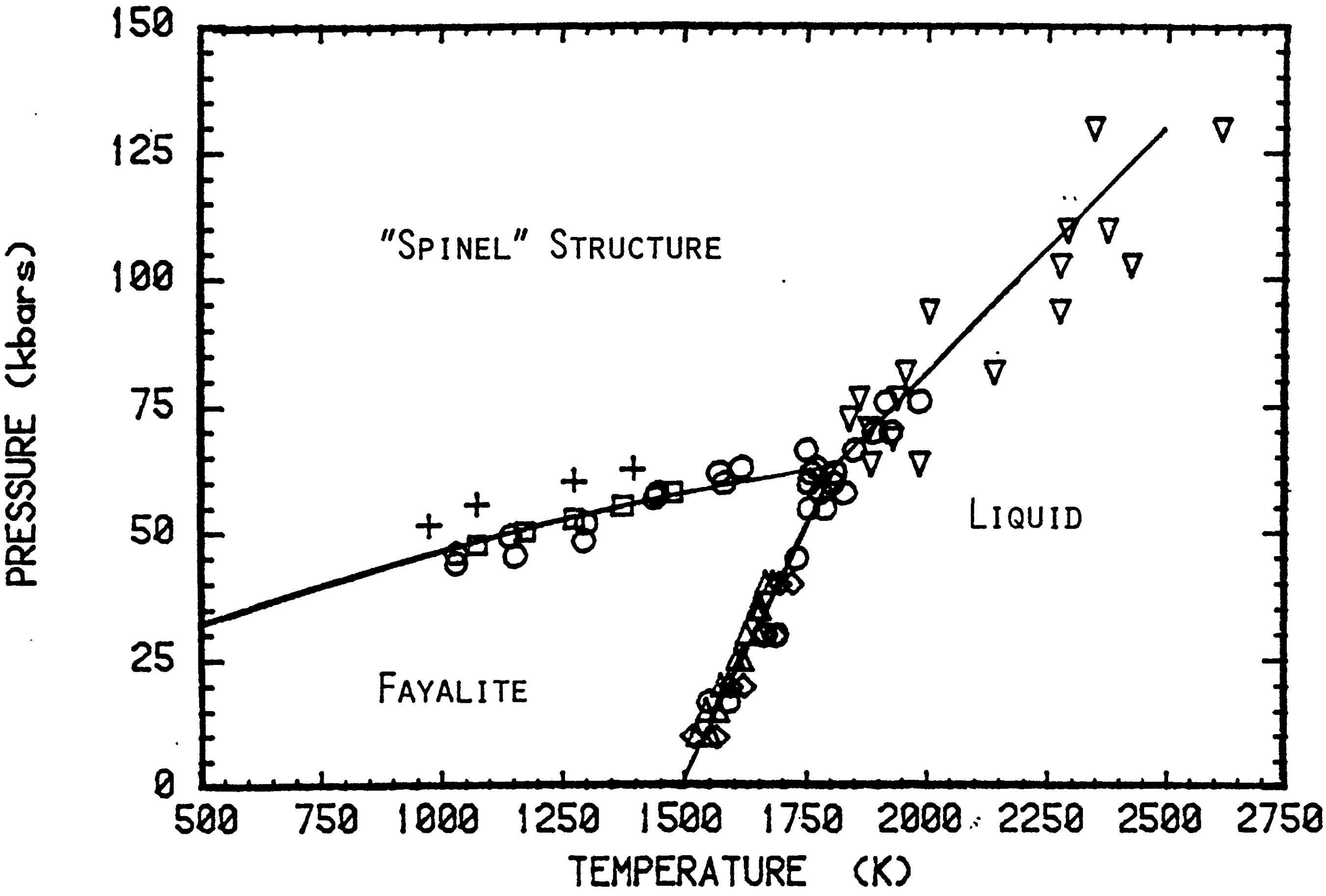
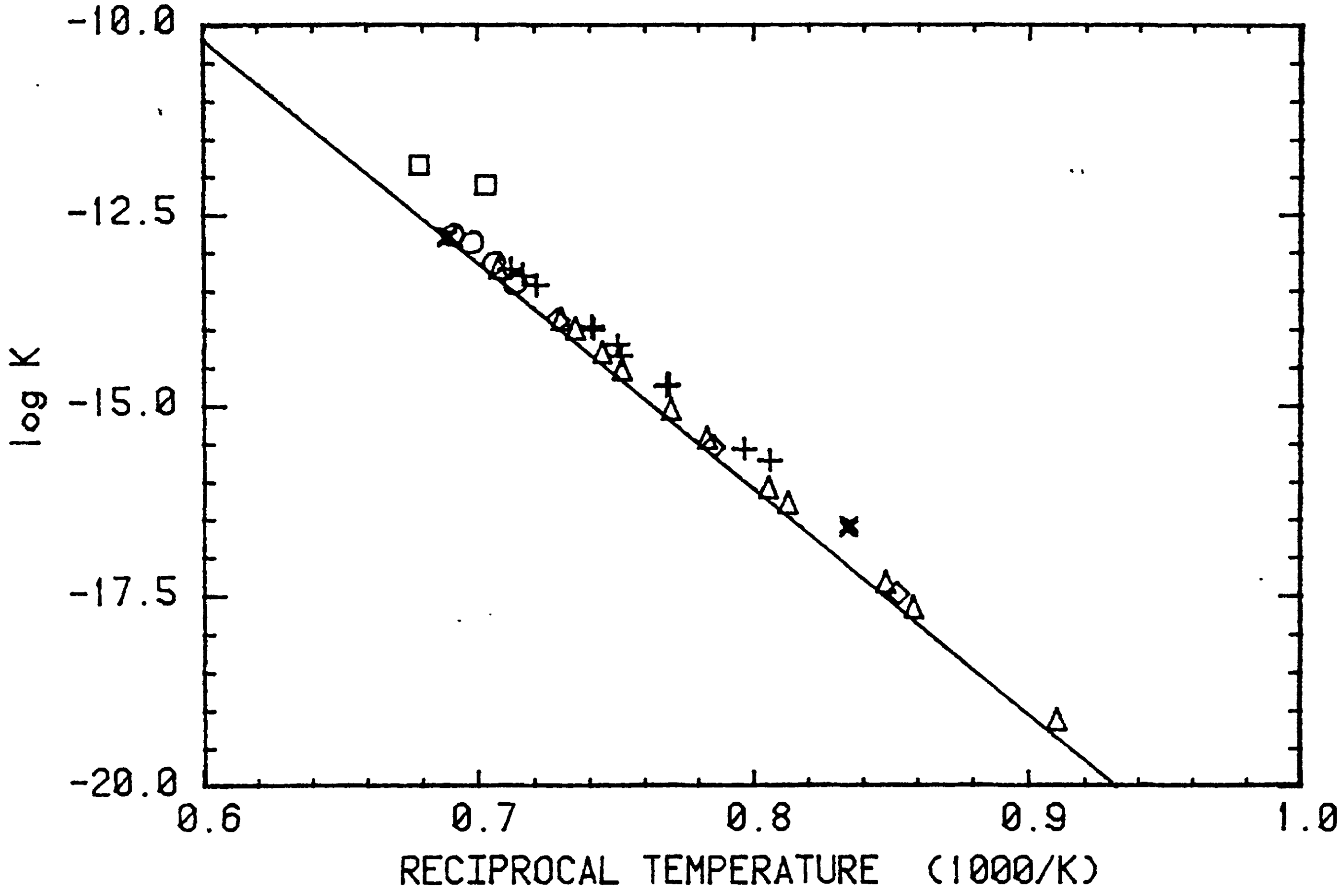


Figure A.60


"SPINEL" STRUCTURE
LIQUID
FAYALITE
PRESSURE (kbars)
0
25
50
75
100
125
150
TEMPERATURE (K)
500
750
1000
1250
1500
1750
2000
2250
2500
2750

J.L. Haas, Jr., "Oxygen Buffers" 1-Dec-87

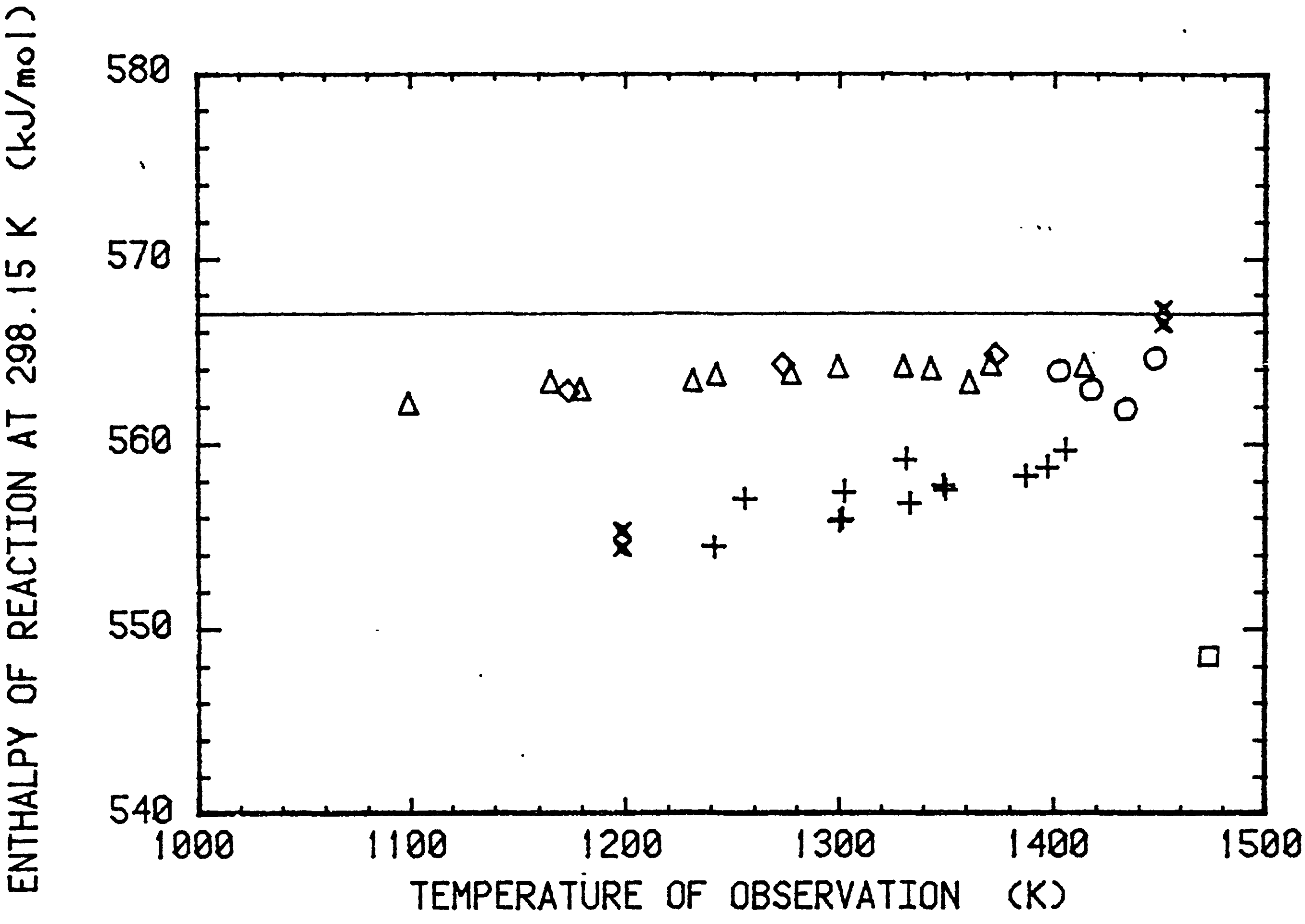
Figure A.61



575

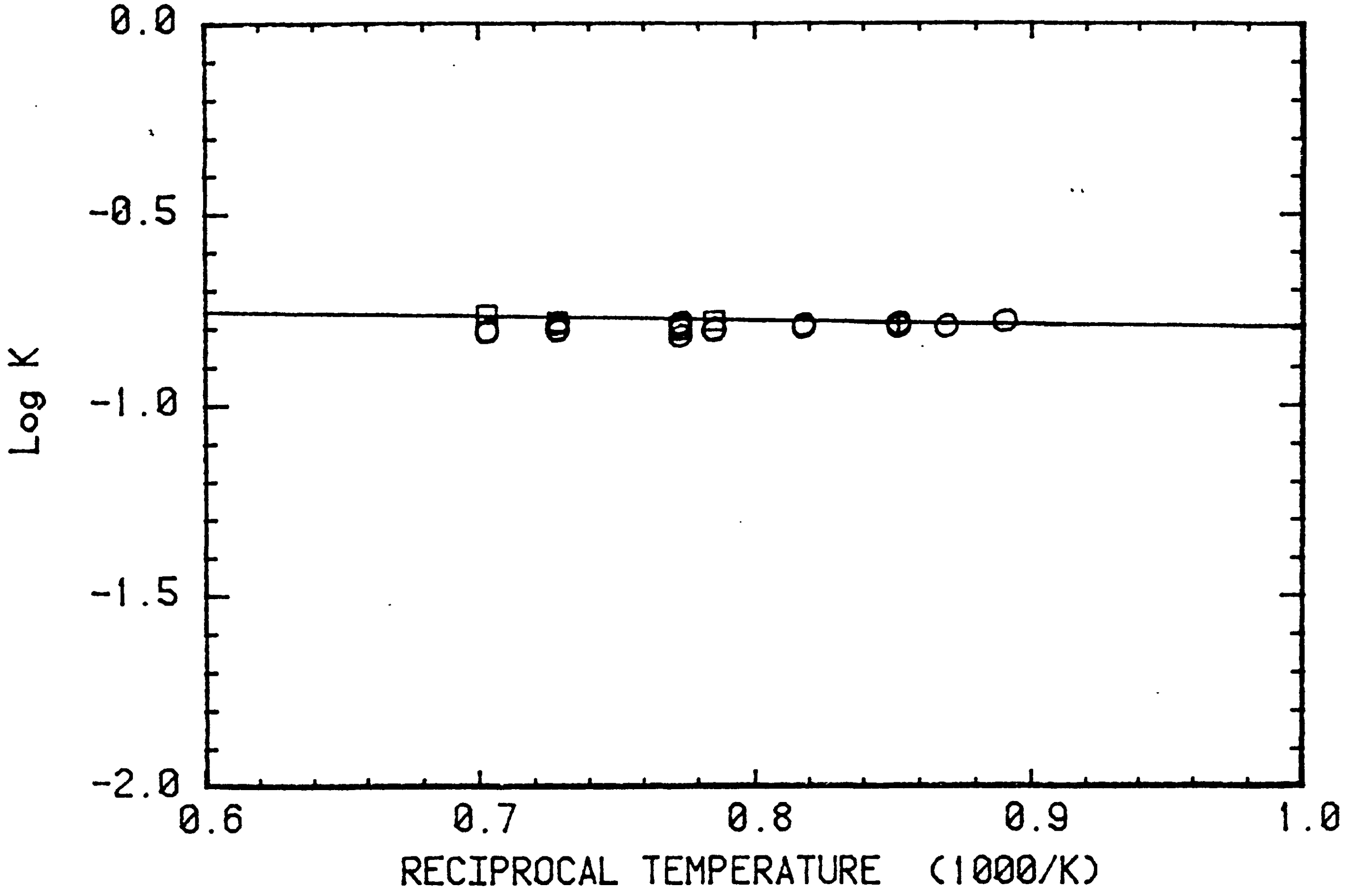
J.L. Haas, Jr., "Oxygen Buffers" 1-Dec-87

Figure A.62



J.L. Haas, Jr., 'Oxygen Buffers' 1-Dec-87

Figure A.63



J.L. Haas, Jr., "Oxygen Buffers" 1-Dec-87

Figure A.64

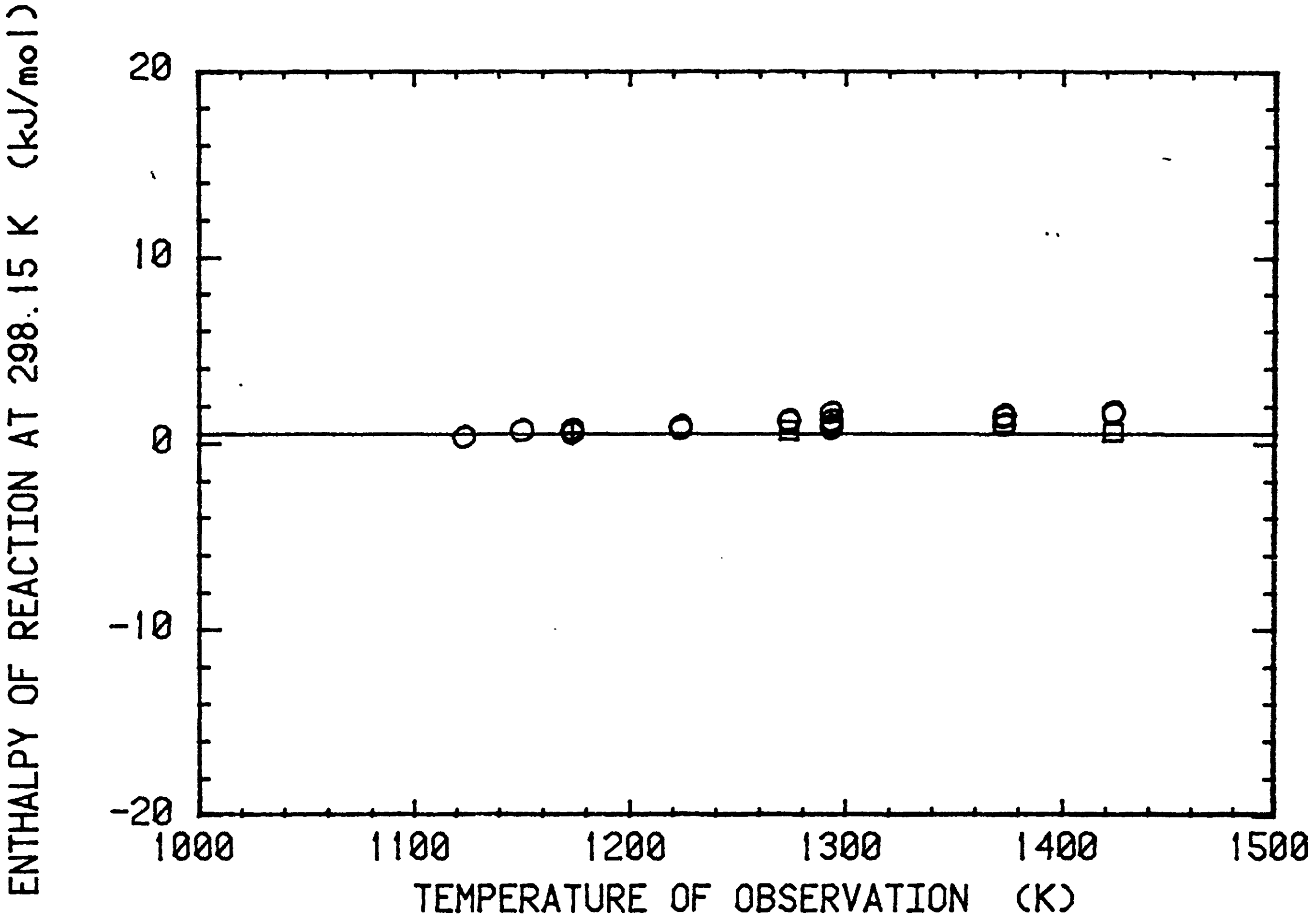


Figure A.65

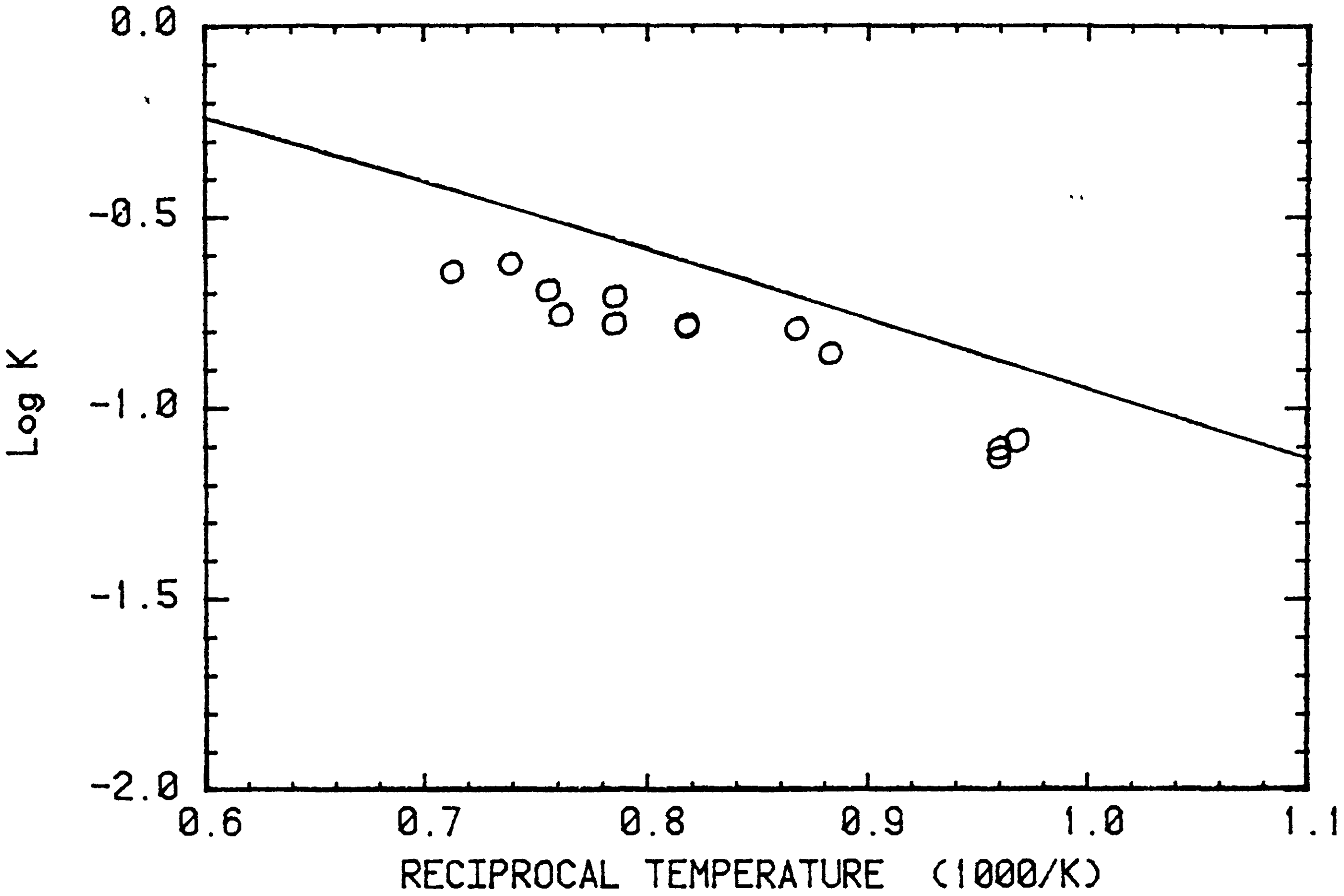
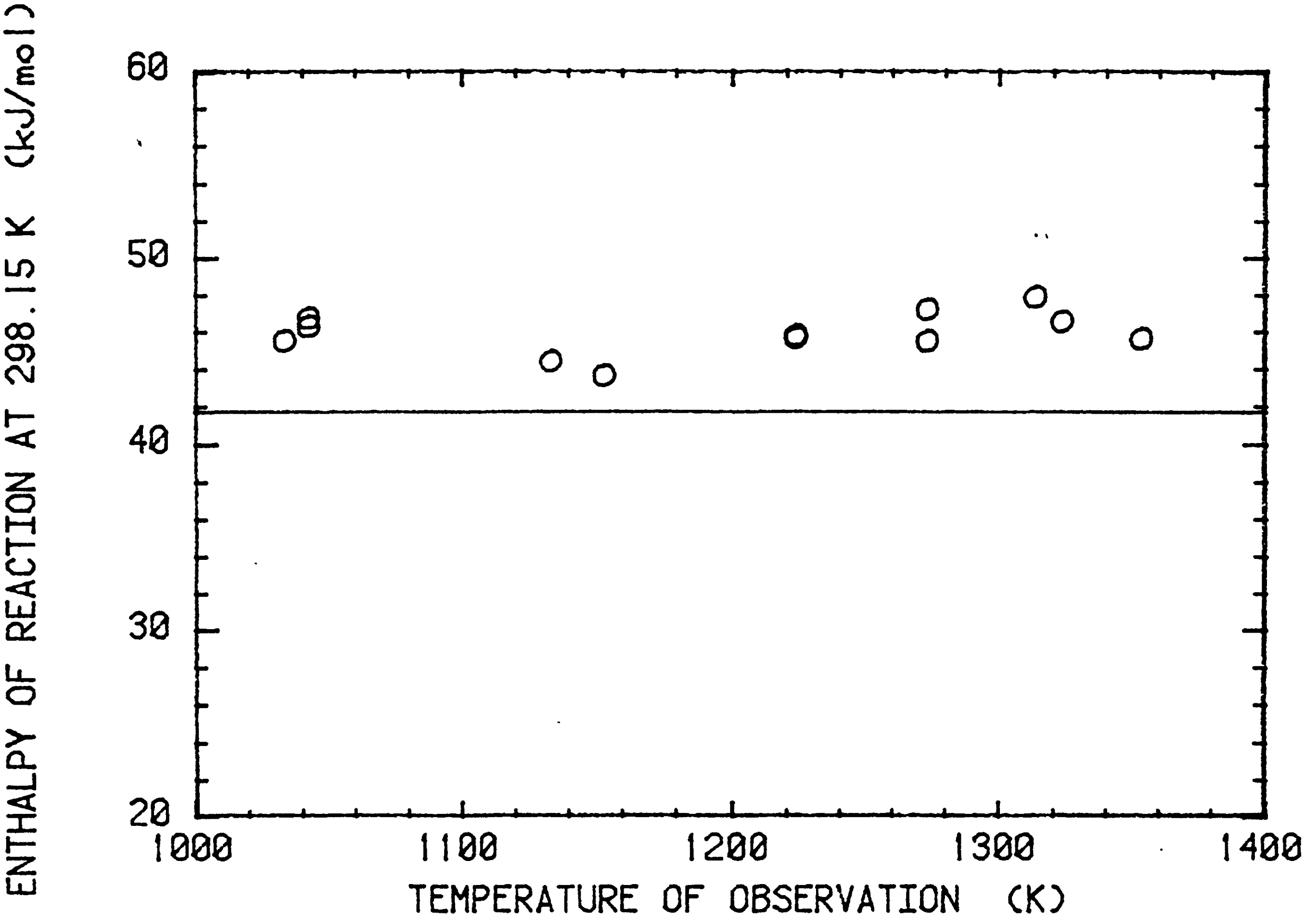

0.0
-0.5
-1.0
-1.5
-2.0
Log K
0.6
0.7
0.8
0.9
1.0
1.1
RECIPROCAL TEMPERATURE (1000/K)

Figure A.66


ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
60
50
40
30
20
1000
1100
1200
1300
1400
TEMPERATURE OF OBSERVATION (K)

J.L. Haas, Jr., 'Oxygen Buffers' 1-Dec-87

Figure A.67

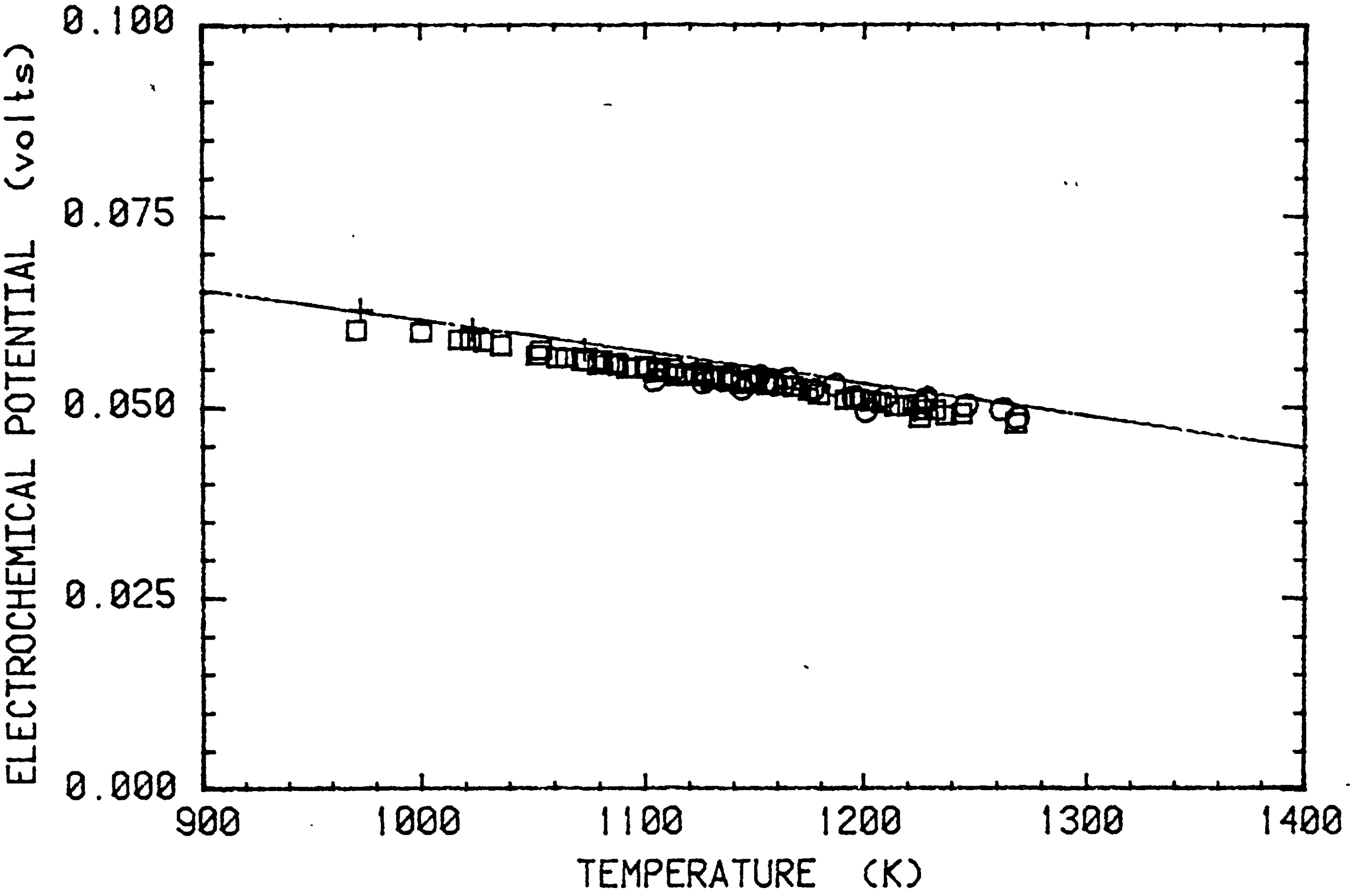
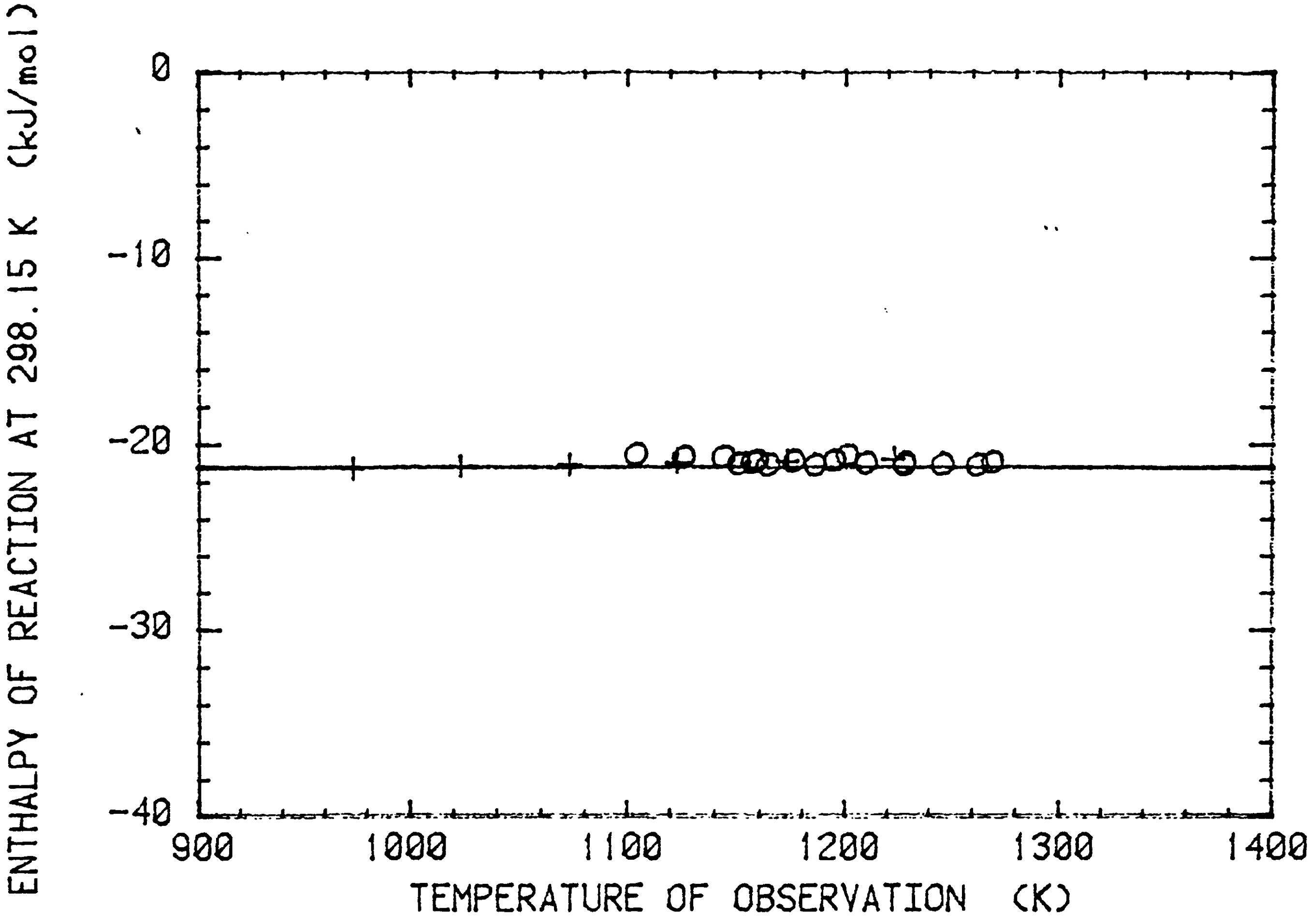


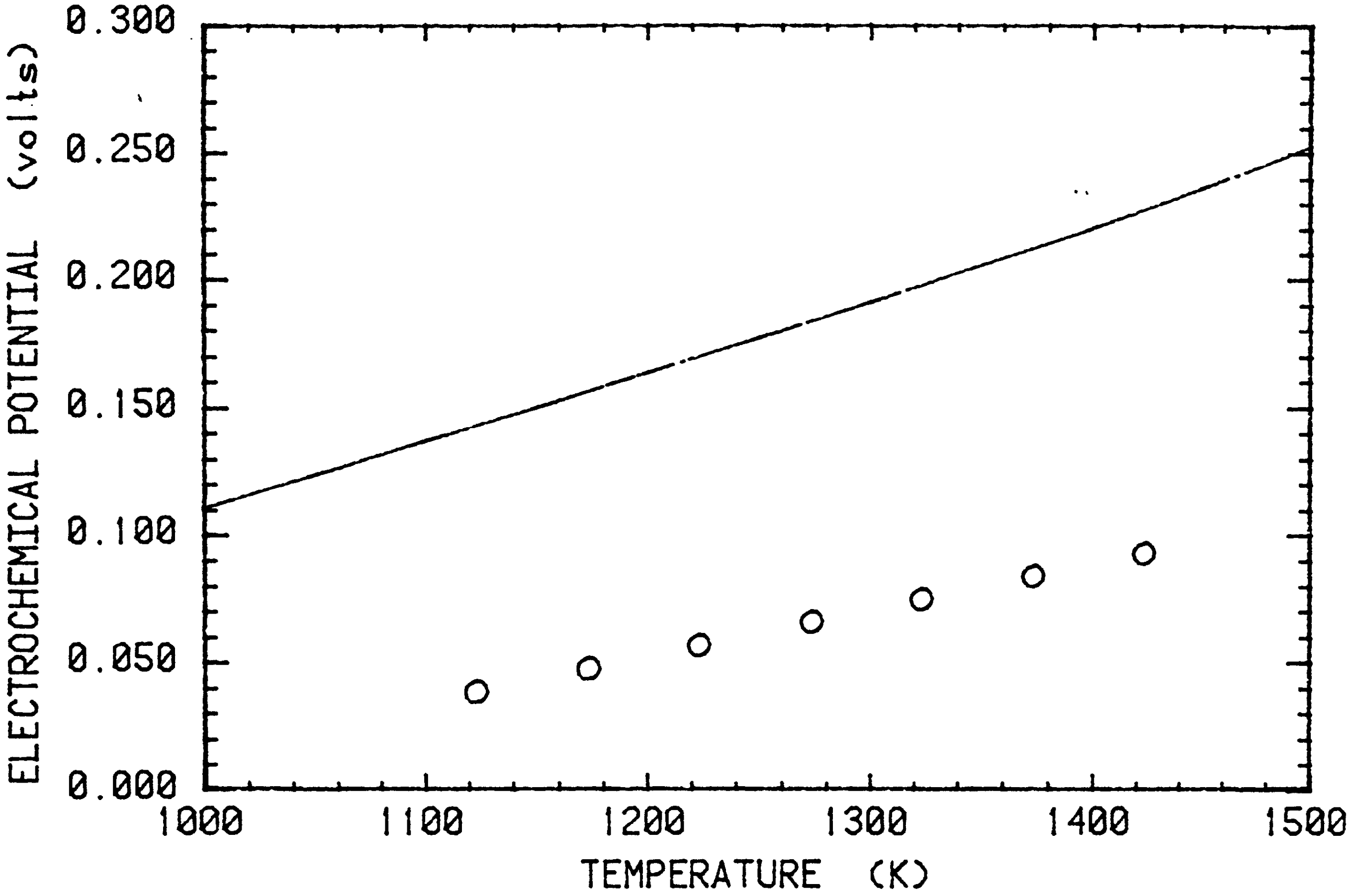
Figure A.68



ENTHALPY OF REACTION AT 298.15 K (kJ/mol)
0
-10
-20
-30
-40
900
1000
1100
1200
1300
1400
TEMPERATURE OF OBSERVATION (K)

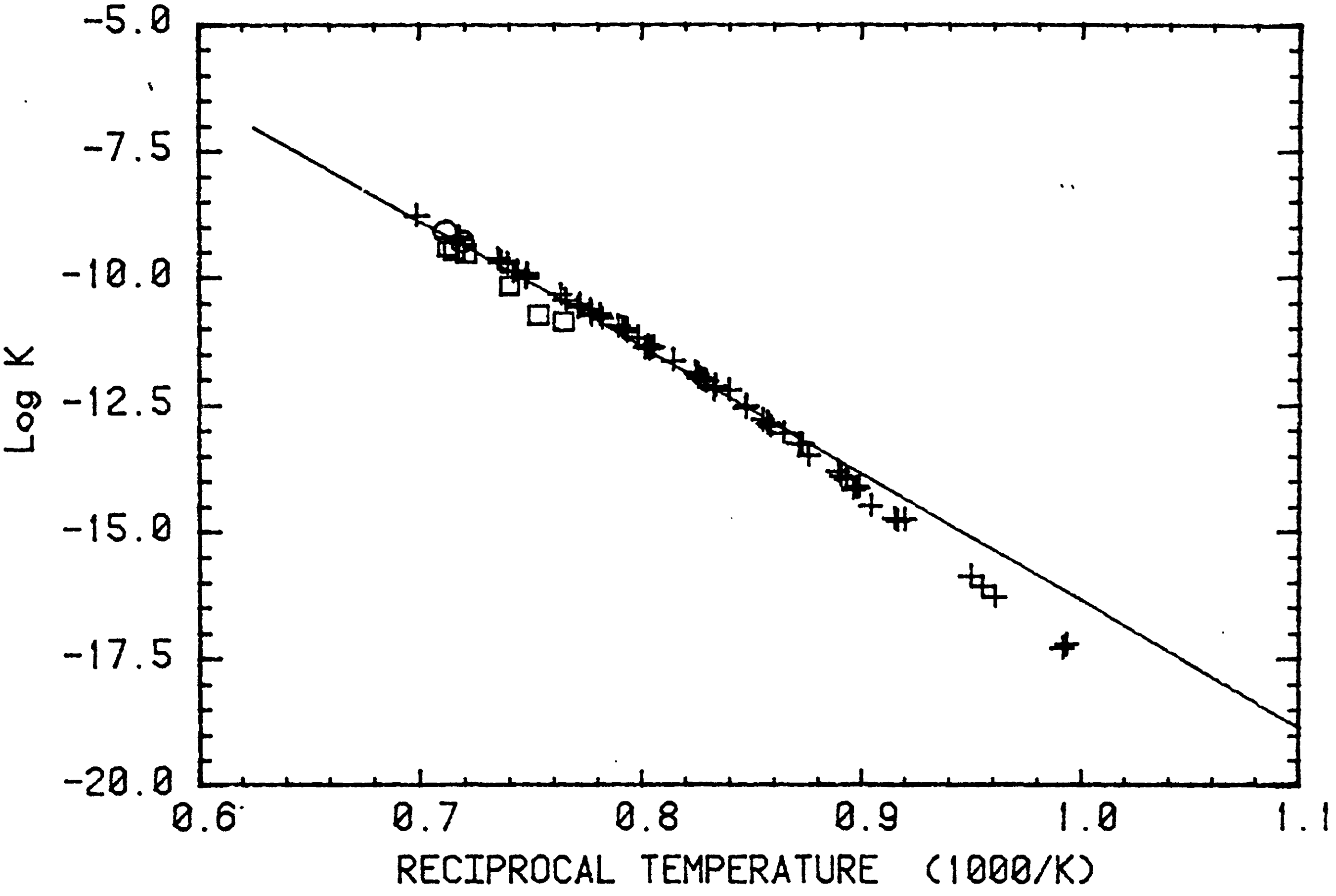
J.L. Haas, Jr., 'Oxygen Buffers' 1-Dec-87

Figure A.69



J.L. Haas, Jr., 'Oxygen Buffers' 1-Dec-87

Figure A.70



J.L. Haas, Jr., 'Oxygen Buffers' 1-Dec-87

Figure A.71

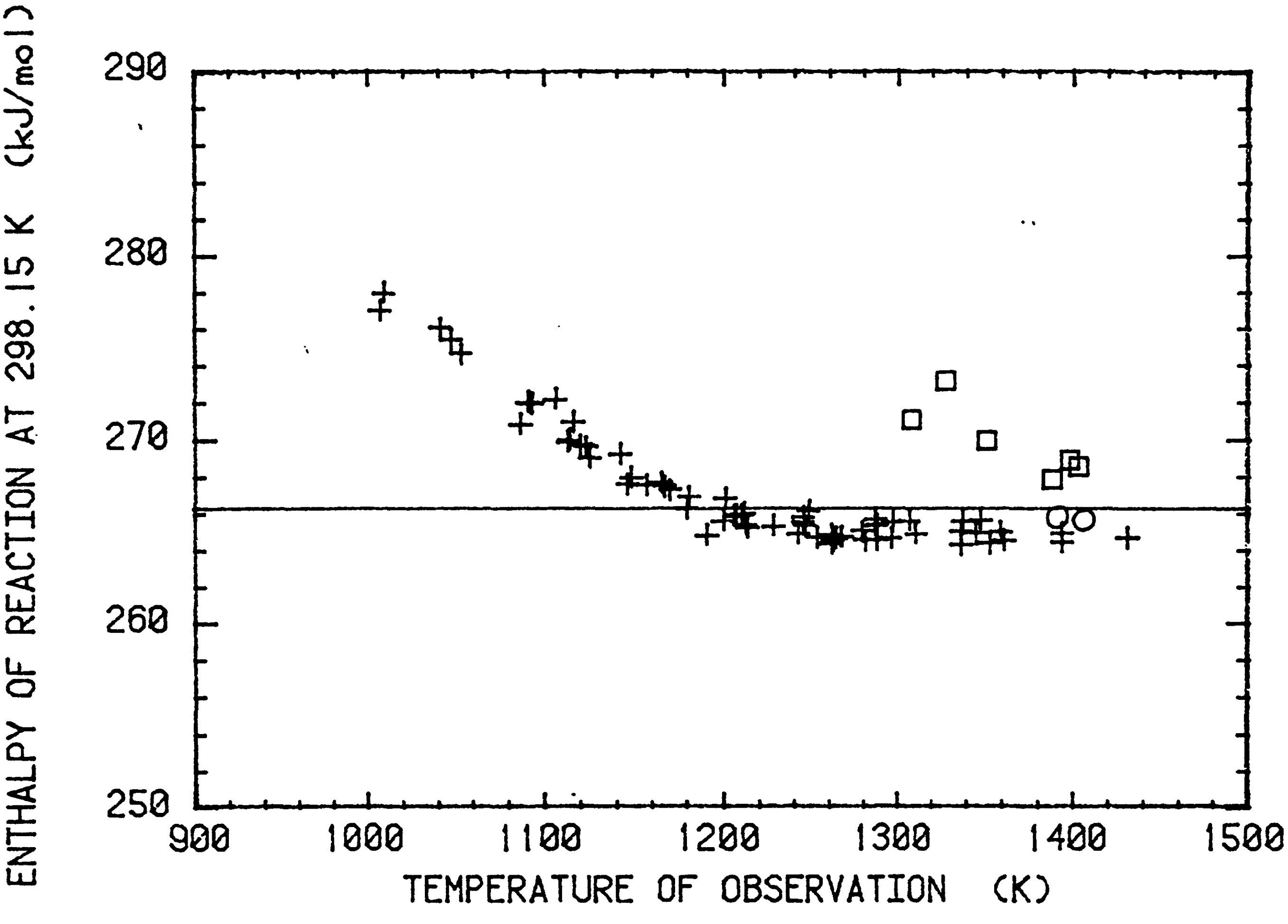


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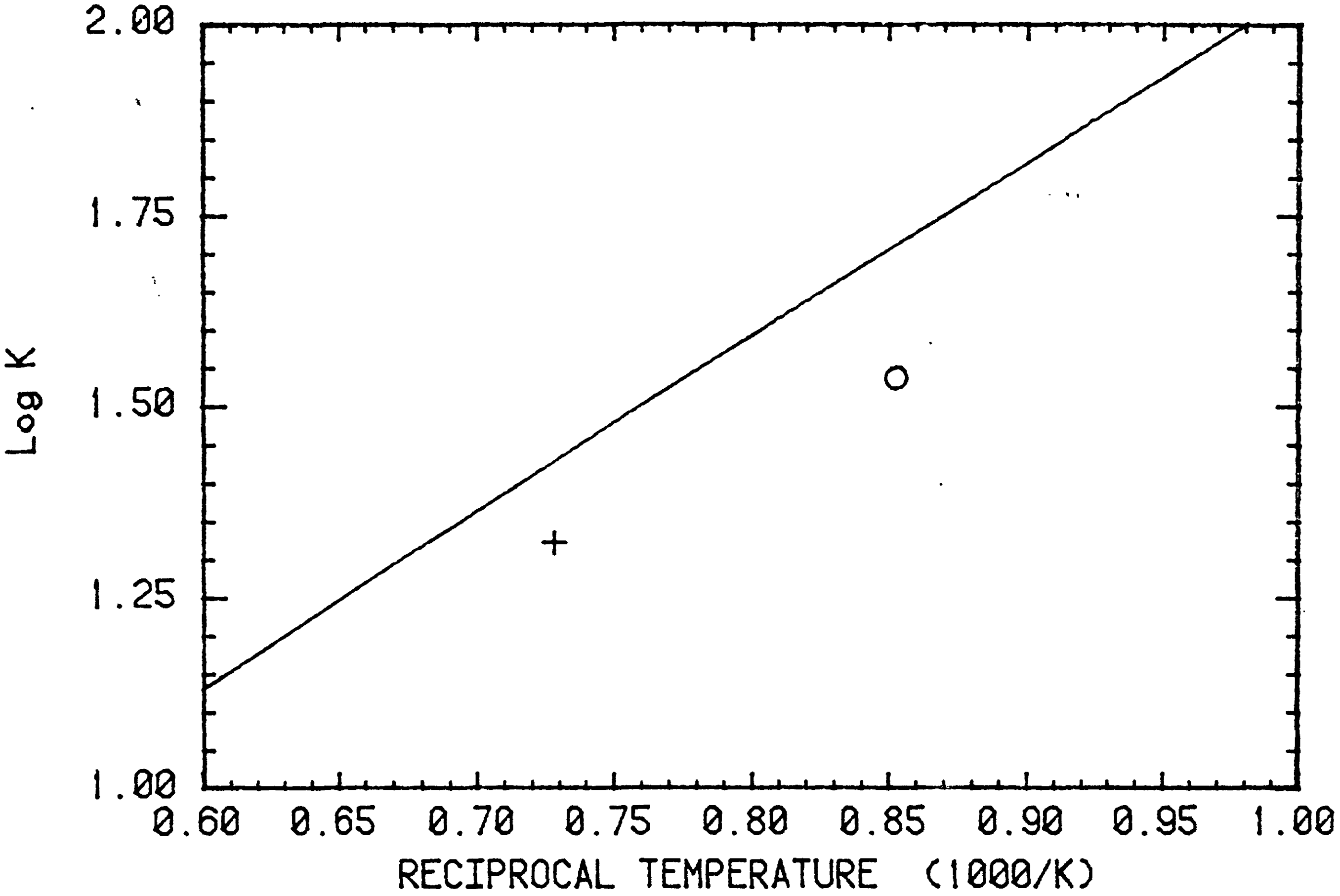
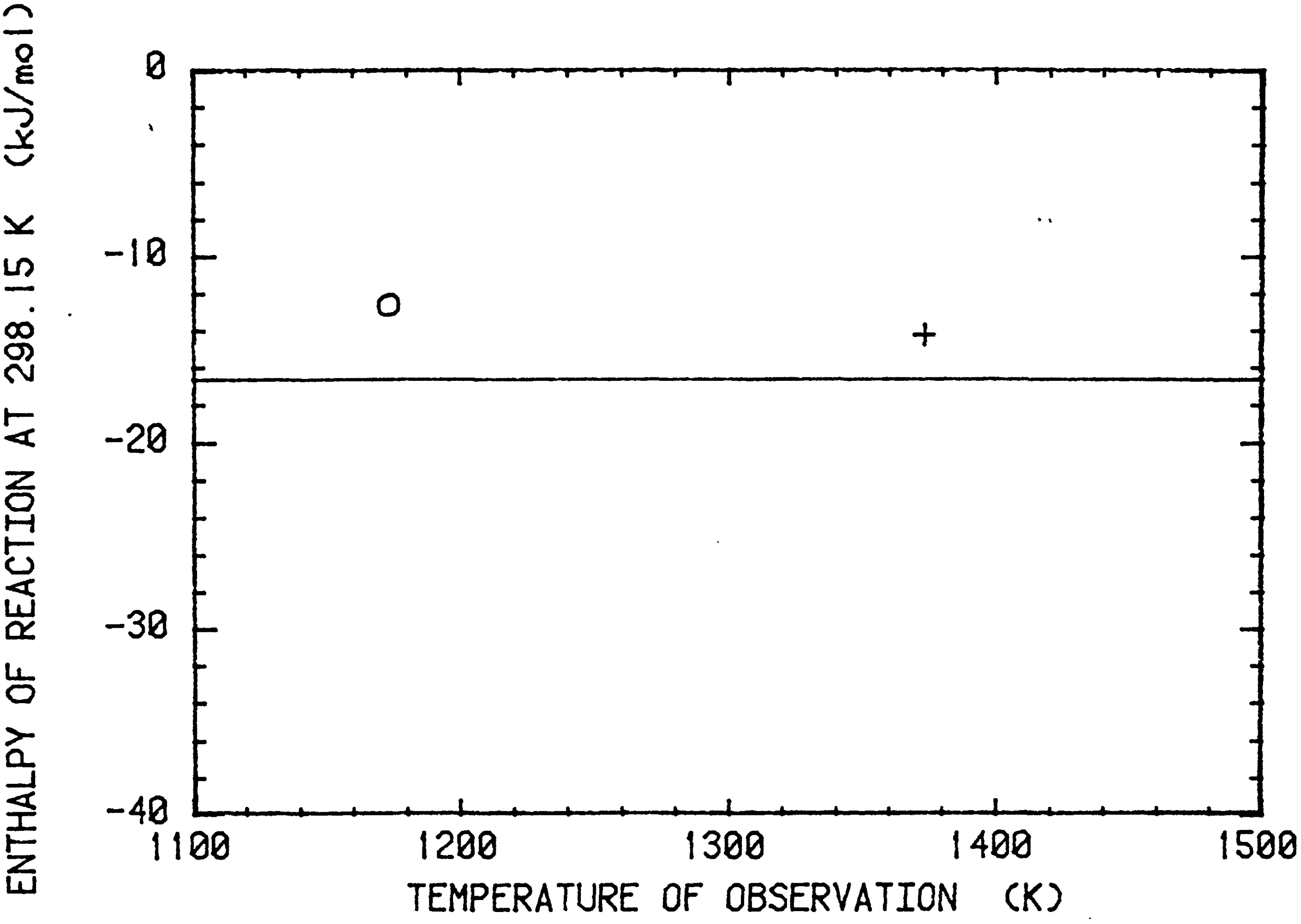
Figure A.72


2.00
1.75
1.50
1.25
1.00
Log K
0.60
0.65
0.70
0.75
0.80
0.85
0.90
0.95
1.00
RECIPROCAL TEMPERATURE (1000/K)

J.L. Haas, Jr., "Oxygen Buffers" 1-Dec-87

Figure A.73



J.L. Haas, Jr., 'Oxygen Buffers' 1-Dec-87

Figure A.74

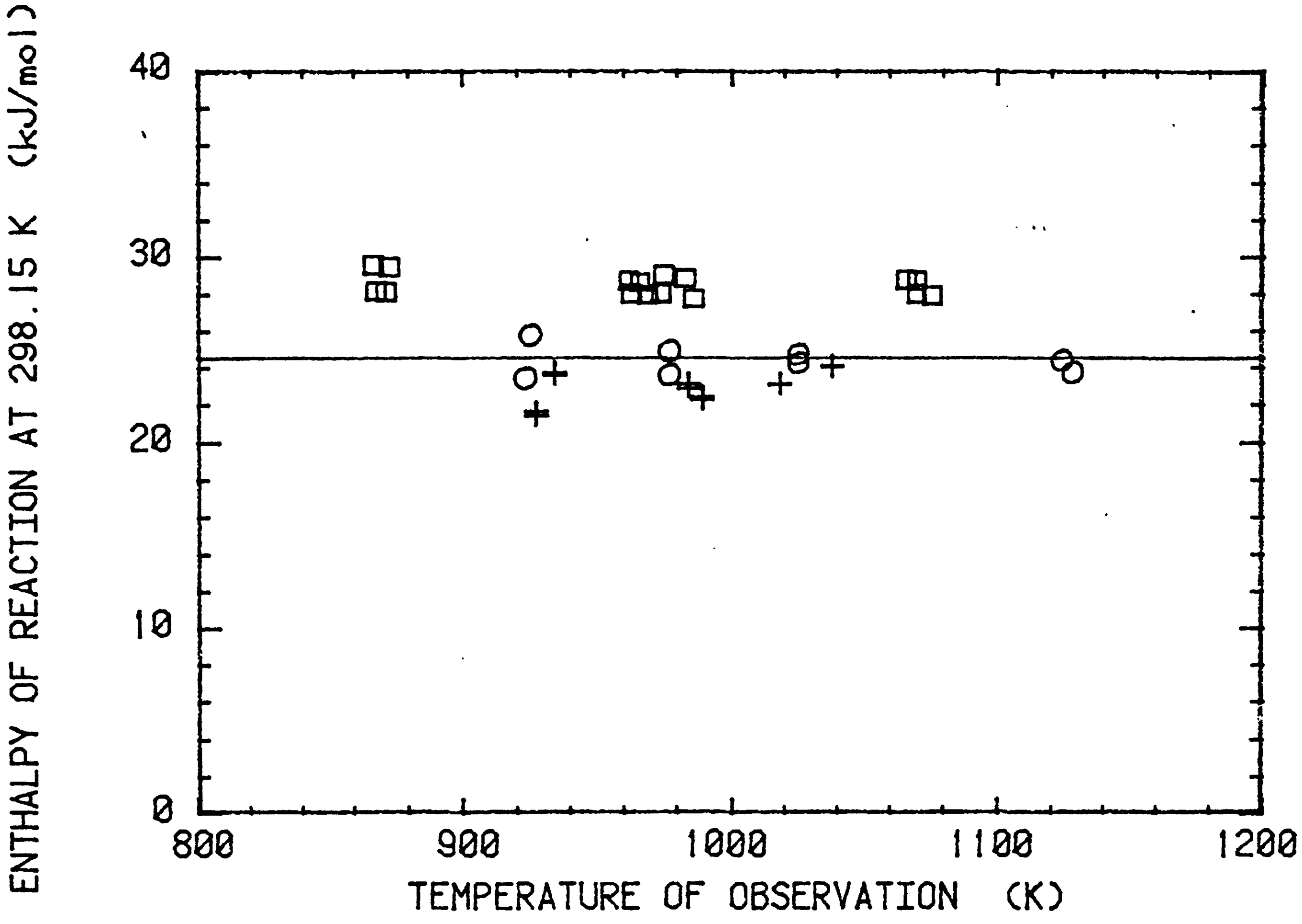
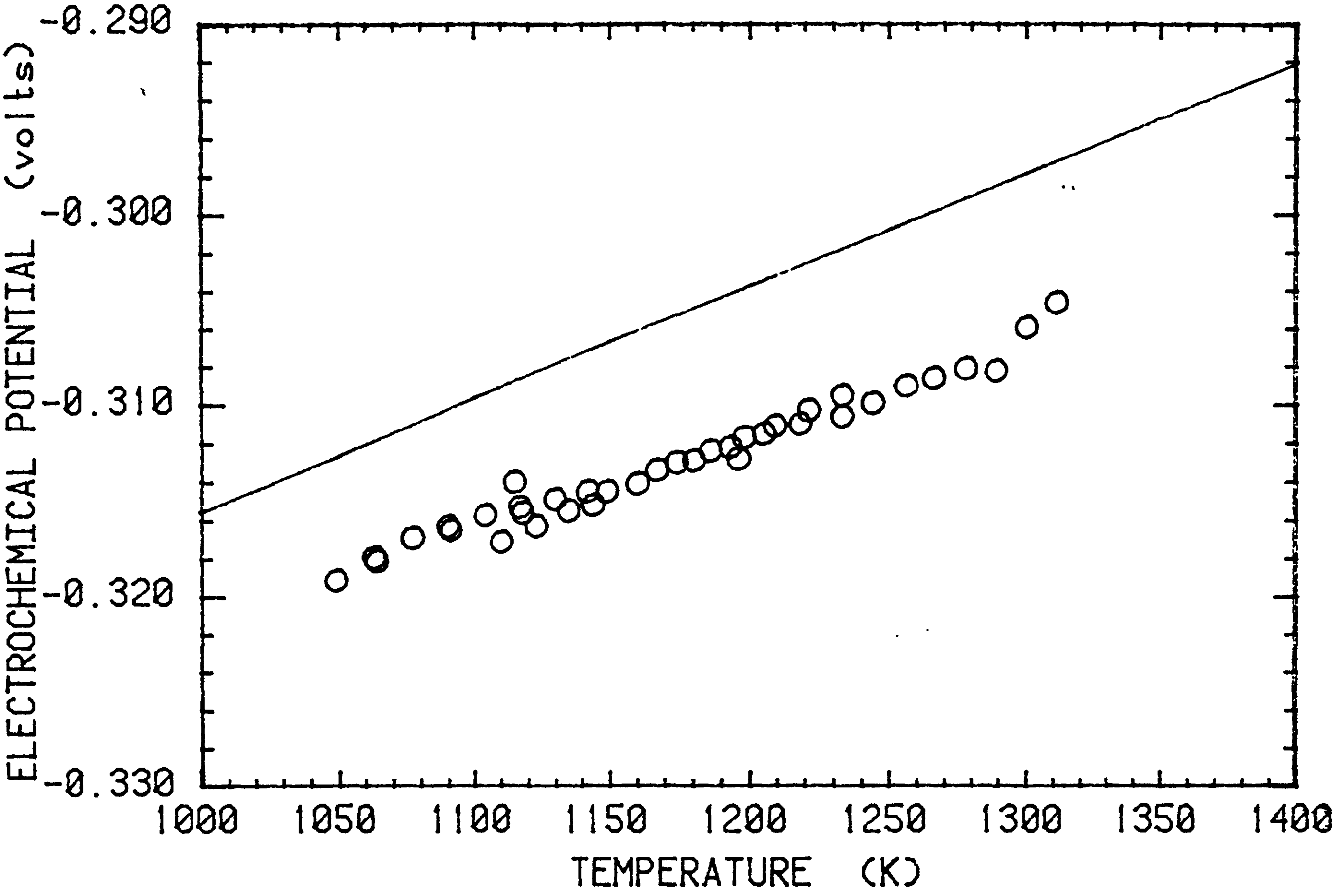
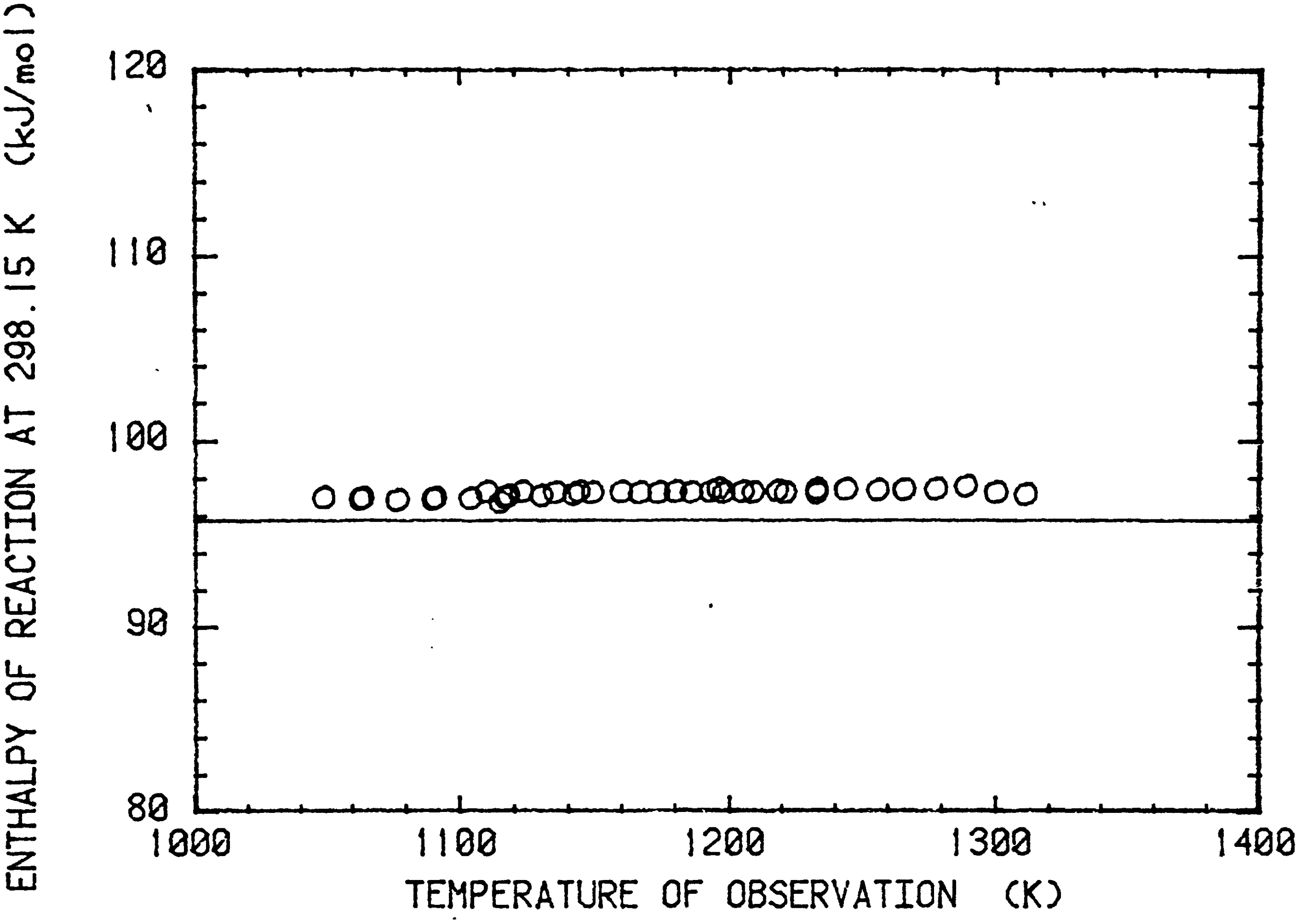


Figure A.75


-0.290
-0.300
-0.310
-0.320
-0.330
1000
1050
1100
1150
1200
1250
1300
1350
1400
ELECTROCHEMICAL POTENTIAL (volts)
TEMPERATURE (K)

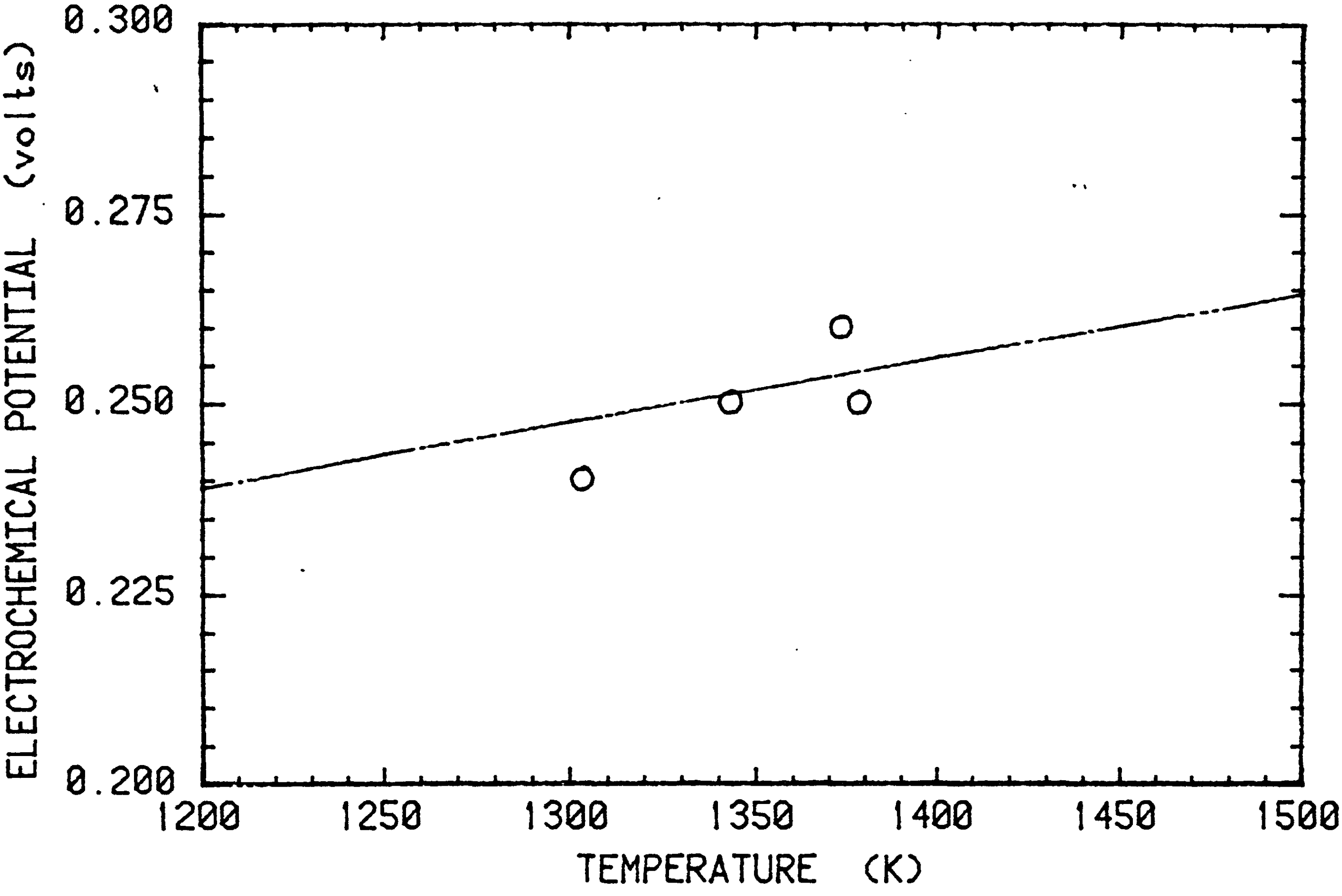
J.L. Haas, Jr., "Oxygen Buffers" 1-Dec-87

Figure A.76



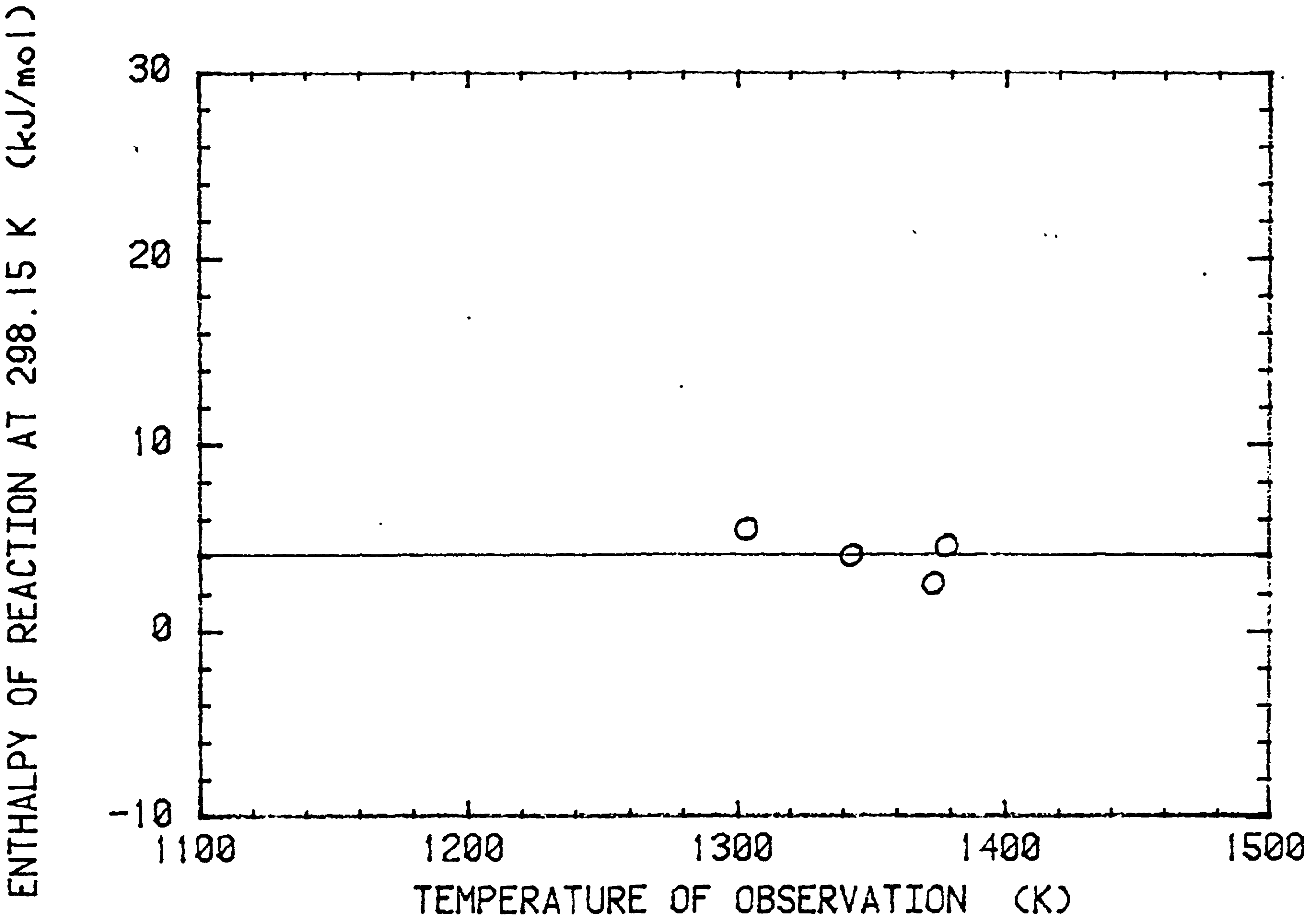
J.L. Haas, Jr., 'Oxygen Buffers' 1-Dec-87

Figure A.77



J.L. Haas, Jr., "Oxygen Buffers" 1 Dec 87

Figure A.78



Recommended Standard Electrochemical Potentials and Fugacities of Oxygen for the Solid Buffers and Thermodynamic Data in the System Iron-Silicon-Oxygen, Nickel-Oxygen, and Copper-Oxygen

Part 5. Revised Tables

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March 6, 1992

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Introduction

The results presented in Tables 8.01 - 8.21 of this section were obtained from computer printouts and computer data files from an analysis of the chemical systems made in early April of 1989. These results reflect changes suggested by the TGCTT and the author of the chapter. The thermodynamic data for the reference phases (e.g., O_2, CO, CO_2) have not changed, but tables are included here for verification of that fact. (References to the source of this data are given in the original tables in Part 2.) The data in these tables are, in the strictest sense, not compatible with the data given for wüstite in Part 2. However, in the practical sense the changes are small and likely within the true experimental error. Thus the data in these tables may be used with the earlier data for wüstite with care.

It should be noted that a separate analysis of iron has been made by Haas and Chase (USGS Open-File Report 89-138) which has been accepted as the CODATA (TGCTT) reference thermodynamic data set for iron. The data for iron used in this report is not the reference data set. Therefore, the evaluation presented here is subject to some additional uncertainty arising from the slight difference in the reference values for iron. A copy of the thermodynamic values for iron compiled from USGS Open-File Report 89-138 are presented here (in a different format) as Table 8-22.

The model used for wüstite was criticized by the TGCTT because it showed wüstite to be stable to lower temperatures than known to be true. The fault of the model was the failure to properly account for the magnetic heat capacity effects in Fe and Fe_3O_4 (see Figure 3.4, Part 4). However, at higher temperatures the model was viewed as providing an excellent representation of wüstite. Attempts to correct the model for the noted deficiency yielded singularity errors in the analysis of the data set, and to subsequent abandonment by Haas of the effort. Thus when the data for wüstite are used, care must be exercised, particularly for values for temperatures less than 900 K.

Table 8.01. Thermodynamic properties of graphite, C(s).

T	V°	S°	$\frac{-(G^\circ_T-H^\circ_{298})}{T}$	$\frac{(H^\circ_T-H^\circ_{298})}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	Δ_fH°	Δ_fG°	$\log {}_fK^\circ$
K	cm^3/mol	-------------J/(mol·K)------------				--------J/mol--------			
200.	----	3.091	6.401	-3.310	5.021	-662.	0.	0.	0.000
250.	----	4.396	5.868	-1.472	6.770	-368.	0.	0.	0.000
273.15	----	5.032	5.770	-0.740	7.610	-202.	0.	0.	0.000
298.15	----	5.738	5.738	0.000	8.513	0.	0.	0.	0.000
300.	----	5.791	5.738	0.053	8.580	16.	0.	0.	0.000
350.	----	7.245	5.849	1.397	10.314	489.	0.	0.	0.000
400.	----	8.728	6.116	2.612	11.906	1045.	0.	0.	0.000
450.	----	10.215	6.489	3.727	13.340	1677.	0.	0.	0.000
500.	----	11.687	6.935	4.752	14.617	2376.	0.	0.	0.000
550.	----	13.135	7.433	5.702	15.751	3136.	0.	0.	0.000
600.	----	14.549	7.968	6.582	16.755	3949.	0.	0.	0.000
650.	----	15.926	8.527	7.398	17.645	4809.	0.	0.	0.000
700.	----	17.263	9.104	8.160	18.433	5712.	0.	0.	0.000
750.	----	18.559	9.691	8.868	19.133	6651.	0.	0.	0.000
800.	----	19.815	10.285	9.530	19.755	7624.	0.	0.	0.000
850.	----	21.029	10.881	10.148	20.309	8626.	0.	0.	0.000
900.	----	22.204	11.478	10.727	20.802	9654.	0.	0.	0.000
950.	----	23.341	12.072	11.268	21.242	10705.	0.	0.	0.000
1000.	----	24.441	12.663	11.777	21.635	11777.	0.	0.	0.000
1050.	----	25.505	13.250	12.255	21.986	12868.	0.	0.	0.000
1100.	----	26.535	13.830	12.705	22.301	13975.	0.	0.	0.000
1150.	----	27.533	14.405	13.128	22.583	15097.	0.	0.	0.000
1200.	----	28.499	14.972	13.528	22.836	16233.	0.	0.	0.000
1250.	----	29.436	15.532	13.905	23.063	17381.	0.	0.	0.000
1300.	----	30.345	16.084	14.261	23.268	18539.	0.	0.	0.000
1350.	----	31.226	16.629	14.598	23.452	19707.	0.	0.	0.000
1400.	----	32.082	17.165	14.917	23.619	20884.	0.	0.	0.000
1450.	----	32.914	17.694	15.220	23.770	22069.	0.	0.	0.000
1500.	----	33.722	18.215	15.507	23.907	23261.	0.	0.	0.000
1550.	----	34.508	18.728	15.780	24.032	24459.	0.	0.	0.000
1600.	----	35.273	19.233	16.040	24.146	25664.	0.	0.	0.000
1650.	----	36.018	19.730	16.287	24.251	26874.	0.	0.	0.000
1700.	----	36.743	20.220	16.523	24.348	28089.	0.	0.	0.000
1750.	----	37.450	20.702	16.747	24.438	29308.	0.	0.	0.000
1800.	----	38.140	21.177	16.962	24.522	30532.	0.	0.	0.000

Table 8.02. Thermodynamic properties of carbon monoxide, CO(g).

T	V°	S°	$\frac{-(G^\circ_T-H^\circ_{298})}{T}$	$\frac{(H^\circ_T-H^\circ_{298})}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log{}_f K^\circ$
K	cm^3/mol	J/(mol·K)				J/mol			
200.	----	186.034	200.326	-14.290	29.028	-2858.	-111291.	-128531.	33.568
250.	----	192.527	198.140	-5.612	29.139	-1403.	-110859.	-132893.	27.766
273.15	----	195.108	197.776	-2.669	29.143	-729.	-110690.	-134941.	25.804
298.15	----	197.660	197.660	0.000	29.146	0.	-110529.	-137168.	24.031
300.	----	197.841	197.661	0.180	29.146	54.	-110518.	-137333.	23.911
350.	----	202.336	198.016	4.320	29.196	1512.	-110270.	-141823.	21.166
400.	----	206.243	198.805	7.438	29.328	2975.	-110110.	-146343.	19.110
450.	----	209.709	199.828	9.880	29.539	4446.	-110029.	-150878.	17.513
500.	----	212.834	200.975	11.860	29.810	5930.	-110016.	-155418.	16.236
550.	----	215.690	202.185	13.505	30.123	7428.	-110062.	-159956.	15.191
600.	----	218.325	203.421	14.905	30.463	8943.	-110158.	-164488.	14.320
650.	----	220.778	204.663	16.115	30.817	10475.	-110295.	-169010.	13.582
700.	----	223.075	205.897	17.177	31.177	12024.	-110467.	-173520.	12.948
750.	----	225.238	207.115	18.123	31.534	13592.	-110668.	-178017.	12.398
800.	----	227.284	208.312	18.973	31.884	15178.	-110894.	-182500.	11.916
850.	----	229.227	209.486	19.741	32.224	16780.	-111140.	-186968.	11.489
900.	----	231.079	210.634	20.444	32.550	18400.	-111404.	-191421.	11.110
950.	----	232.847	211.757	21.089	32.862	20035.	-111682.	-195859.	10.769
1000.	----	234.540	212.854	21.686	33.158	21686.	-111972.	-200282.	10.461
1050.	----	236.165	213.926	22.239	33.438	23351.	-112272.	-204690.	10.183
1100.	----	237.726	214.973	22.754	33.700	25029.	-112581.	-209084.	9.928
1150.	----	239.230	215.995	23.235	33.946	26720.	-112897.	-213463.	9.696
1200.	----	240.680	216.993	23.687	34.175	28424.	-113220.	-217829.	9.482
1250.	----	242.079	217.969	24.110	34.388	30138.	-113548.	-222181.	9.284
1300.	----	243.432	218.922	24.509	34.584	31862.	-113880.	-226519.	9.101
1350.	----	244.740	219.854	24.886	34.765	33596.	-114217.	-230845.	8.932
1400.	----	246.008	220.766	25.241	34.930	35338.	-114558.	-235159.	8.774
1450.	----	247.236	221.658	25.579	35.080	37089.	-114902.	-239460.	8.626
1500.	----	248.428	222.530	25.897	35.216	38846.	-115250.	-243749.	8.488
1550.	----	249.584	223.384	26.200	35.338	40610.	-115600.	-248026.	8.358
1600.	----	250.708	224.221	26.487	35.446	42380.	-115954.	-252292.	8.236
1650.	----	251.800	225.040	26.760	35.542	44154.	-116311.	-256548.	8.121
1700.	----	252.863	225.843	27.020	35.625	45934.	-116671.	-260792.	8.013
1750.	----	253.896	226.630	27.267	35.696	47717.	-117035.	-265025.	7.910
1800.	----	254.903	227.401	27.502	35.755	49503.	-117402.	-269248.	7.813

Table 8.03. Thermodynamic properties of carbon dioxide, $CO_2(g)$.

T	V°	S°	$\frac{-(G^\circ_T-H^\circ_{298})}{T}$	$\frac{(H^\circ_T-H^\circ_{298})}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log_f K^\circ$
K	cm^3/mol	-------------J/(mol·K)------------				--------J/mol--------			
200.	----	199.965	217.032	-17.065	32.226	-3413.	-393392.	-394070.	102.918
250.	----	207.446	214.385	-6.940	34.866	-1735.	-393465.	-394230.	82.368
273.15	----	210.583	213.931	-3.346	35.990	-914.	-393489.	-394300.	75.401
298.15	----	213.786	213.786	0.000	37.148	0.	-393510.	-394373.	69.091
300.	----	214.016	213.786	0.230	37.231	69.	-393511.	-394378.	68.666
350.	----	219.918	214.248	5.671	39.375	1985.	-393543.	-394520.	58.878
400.	----	225.305	215.298	10.008	41.311	4003.	-393574.	-394658.	51.536
450.	----	230.273	216.689	13.584	43.059	6113.	-393612.	-394791.	45.825
500.	----	234.893	218.281	16.612	44.635	8306.	-393661.	-394920.	41.256
550.	----	239.215	219.990	19.225	46.060	10574.	-393722.	-395043.	37.517
600.	----	243.279	221.763	21.517	47.350	12910.	-393793.	-395160.	34.401
650.	----	247.116	223.567	23.549	48.520	15307.	-393873.	-395271.	31.764
700.	----	250.751	225.380	25.371	49.585	17760.	-393961.	-395375.	29.503
750.	----	254.206	227.188	27.019	50.555	20264.	-394056.	-395473.	27.543
800.	----	257.497	228.980	28.518	51.441	22814.	-394156.	-395564.	25.827
850.	----	260.641	230.751	29.891	52.252	25407.	-394260.	-395649.	24.313
900.	----	263.649	232.495	31.153	52.995	28038.	-394366.	-395727.	22.967
950.	----	266.533	234.211	32.321	53.677	30705.	-394475.	-395800.	21.762
1000.	----	269.302	235.897	33.405	54.304	33405.	-394584.	-395867.	20.678
1050.	----	271.966	237.552	34.414	54.881	36135.	-394694.	-395928.	19.696
1100.	----	274.531	239.175	35.356	55.412	38892.	-394804.	-395984.	18.803
1150.	----	277.005	240.766	36.239	55.902	41675.	-394914.	-396035.	17.988
1200.	----	279.394	242.326	37.068	56.353	44482.	-395023.	-396082.	17.241
1250.	----	281.703	243.855	37.848	56.770	47310.	-395132.	-396124.	16.553
1300.	----	283.937	245.354	38.583	57.153	50158.	-395239.	-396161.	15.918
1350.	----	286.101	246.823	39.278	57.507	53025.	-395346.	-396195.	15.329
1400.	----	288.198	248.264	39.934	57.834	55908.	-395451.	-396224.	14.783
1450.	----	290.233	249.676	40.557	58.134	58808.	-395556.	-396250.	14.274
1500.	----	292.209	251.061	41.147	58.411	61721.	-395660.	-396272.	13.799
1550.	----	294.128	252.420	41.708	58.665	64648.	-395764.	-396291.	13.355
1600.	----	295.994	253.752	42.242	58.899	67588.	-395867.	-396306.	12.938
1650.	----	297.810	255.060	42.750	59.113	70538.	-395970.	-396318.	12.546
1700.	----	299.578	256.343	43.235	59.309	73499.	-396073.	-396327.	12.177
1750.	----	301.300	257.603	43.697	59.488	76469.	-396177.	-396333.	11.830
1800.	----	302.978	258.841	44.137	59.651	79447.	-396281.	-396336.	11.501

Table 8.04. Thermodynamic properties of copper, Cu(s,l).

T K	V° cm^3/mol	S°	$-\frac{(G^\circ_T-H^\circ_{298})}{T}$	$\frac{(H^\circ_T-H^\circ_{298})}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log_f K^\circ$
		-------------J/(mol·K)			------------	--------J/mol		--------	
200.	----	23.732	35.325	-11.595	22.668	-2319.	0.	0.	0.000
250.	----	28.902	33.539	-4.636	23.676	-1159.	0.	0.	0.000
273.15	----	31.016	33.236	-2.219	24.068	-606.	0.	0.	0.000
298.15	----	33.140	33.140	0.000	24.436	0.	0.	0.	0.000
300.	----	33.292	33.141	0.150	24.461	45.	0.	0.	0.000
350.	----	37.108	33.441	3.666	25.032	1283.	0.	0.	0.000
400.	----	40.478	34.114	6.365	25.440	2546.	0.	0.	0.000
450.	----	43.493	34.992	8.502	25.740	3826.	0.	0.	0.000
500.	----	46.218	35.980	10.238	25.978	5119.	0.	0.	0.000
550.	----	48.703	37.026	11.678	26.184	6423.	0.	0.	0.000
600.	----	50.990	38.095	12.895	26.383	7737.	0.	0.	0.000
650.	----	53.110	39.170	13.940	26.589	9061.	0.	0.	0.000
700.	----	55.089	40.237	14.851	26.814	10396.	0.	0.	0.000
750.	----	56.947	41.290	15.657	27.065	11743.	0.	0.	0.000
800.	----	58.703	42.324	16.379	27.345	13103.	0.	0.	0.000
850.	----	60.369	43.336	17.033	27.657	14478.	0.	0.	0.000
900.	----	61.960	44.327	17.632	28.002	15869.	0.	0.	0.000
950.	----	63.484	45.296	18.188	28.381	17279.	0.	0.	0.000
1000.	----	64.950	46.242	18.708	28.794	18708.	0.	0.	0.000
1050.	----	66.366	47.167	19.199	29.240	20159.	0.	0.	0.000
1100.	----	67.737	48.071	19.666	29.718	21633.	0.	0.	0.000
1150.	----	69.069	48.955	20.114	30.228	23131.	0.	0.	0.000
1200.	----	70.367	49.820	20.547	30.767	24656.	0.	0.	0.000
1250.	----	71.634	50.667	20.966	31.336	26208.	0.	0.	0.000
1300.	----	72.875	51.498	21.377	31.933	27790.	0.	0.	0.000
1350.	----	74.091	52.312	21.779	32.556	29402.	0.	0.	0.000
1357.6	----	74.274	52.434	21.840	32.653	29650.	0.	0.	0.000
				Crystal = Liquid					
1357.6	----	83.941	52.434	31.506	32.800	42773.	0.	0.	0.000
1400.	----	84.950	53.404	31.546	32.800	44164.	0.	0.	0.000
1450.	----	86.101	54.512	31.589	32.800	45804.	0.	0.	0.000
1500.	----	87.213	55.583	31.629	32.800	47444.	0.	0.	0.000
1550.	----	88.288	56.621	31.667	32.800	49084.	0.	0.	0.000
1600.	----	89.330	57.627	31.703	32.800	50724.	0.	0.	0.000
1650.	----	90.339	58.603	31.736	32.800	52364.	0.	0.	0.000
1700.	----	91.318	59.551	31.767	32.800	54004.	0.	0.	0.000
1750.	----	92.269	60.472	31.797	32.800	55644.	0.	0.	0.000
1800.	----	93.193	61.368	31.824	32.800	57284.	0.	0.	0.000

Table 8.05. Thermodynamic properties of tenorite, CuO(s).

T	V°	S°	$-(G^\circ_T-H^\circ_{298})/T$	$(H^\circ_T-H^\circ_{298})/T$	C°_p	$H^\circ_T-H^\circ_{298}$	Δ_fH°	Δ_fG°	$\log {}_fK^\circ$
K	cm³/mol	J/(mol·K)				J/mol			
200.	----	27.019	46.271	-19.250	34.859	-3850.	-155711.	-137020.	35.785
227.	----	31.722	44.261	-12.537	39.566	-2846.	-155719.	-134495.	30.948
2 s	----	0.086	0.091	-0.079	0.525	18.	205.	200.	0.046
					T_N				
227.	----	31.722	44.261	-12.537	39.566	-2846.	-155719.	-134495.	30.948
250.	----	35.457	43.282	-7.824	39.088	-1956.	-155705.	-132345.	27.651
2 s	----	0.086	0.088	0.060	0.261	15.	205.	199.	0.042
273.15	----	38.983	42.769	-3.785	40.575	-1034.	-155675.	-130183.	24.895
298.15	----	42.605	42.605	0.000	42.149	0.	-155614.	-127853.	22.399
2 s	----	0.086	0.086	0.000	0.365	0.	209.	198.	0.035
300.	----	42.866	42.606	0.260	42.259	78.	-155608.	-127680.	22.231
350.	----	49.585	43.130	6.454	44.858	2259.	-155403.	-123041.	18.362
400.	----	55.709	44.326	11.383	46.814	4553.	-155117.	-118436.	15.466
450.	----	61.312	45.906	15.407	48.294	6933.	-154776.	-113871.	13.218
500.	----	66.462	47.708	18.754	49.441	9377.	-154396.	-109346.	11.423
2 s	----	0.204	0.103	0.132	0.349	66.	257.	182.	0.019
550.	----	71.219	49.632	21.587	50.356	11873.	-153989.	-104861.	9.959
600.	----	75.634	51.617	24.017	51.111	14410.	-153563.	-100413.	8.742
650.	----	79.751	53.624	26.126	51.756	16982.	-153123.	-96002.	7.715
700.	----	83.607	55.630	27.977	52.324	19584.	-152676.	-91625.	6.837
750.	----	87.235	57.617	29.619	52.842	22214.	-152223.	-87280.	6.079
2 s	----	0.264	0.134	0.176	0.525	132.	316.	141.	0.010
800.	----	90.661	59.576	31.085	53.327	24868.	-151767.	-82965.	5.417
850.	----	93.908	61.501	32.407	53.792	27546.	-151311.	-78679.	4.835
900.	----	96.996	63.388	33.608	54.246	30247.	-150857.	-74419.	4.319
950.	----	99.941	65.235	34.706	54.696	32971.	-150405.	-70185.	3.859
1000.	----	102.758	67.041	35.717	55.146	35717.	-149956.	-65975.	3.446
2 s	----	0.295	0.157	0.194	0.510	194.	347.	96.	0.005
1050.	----	105.459	68.807	36.652	55.600	38485.	-149513.	-61787.	3.074
1100.	----	108.056	70.532	37.525	56.062	41277.	-149075.	-57619.	2.736
1150.	----	110.559	72.218	38.341	56.532	44092.	-148644.	-53472.	2.429
1200.	----	112.975	73.867	39.108	57.012	46930.	-148221.	-49343.	2.148
1250.	----	115.312	75.478	39.834	57.502	49793.	-147805.	-45232.	1.890
2 s	----	0.280	0.171	0.192	1.535	240.	336.	91.	0.004
1300.	----	117.577	77.054	40.524	58.005	52681.	-147398.	-41137.	1.653
1350.	----	119.776	78.595	41.181	58.519	55594.	-146999.	-37058.	1.434
1357.6	----	120.105	78.827	41.278	58.598	56039.	-146939.	-36439.	1.402
2 s	----	0.336	0.173	0.275	2.224	374.	417.	103.	0.004
				Cu(Crystal = Liquid)					
1357.6	----	120.105	78.827	41.278	58.598	56039.	-160063.	-36439.	1.402
1400.	----	121.914	80.105	41.809	59.044	58533.	-159728.	-32583.	1.216
1450.	----	123.995	81.582	42.412	59.582	61498.	-159312.	-28049.	1.010
1500.	----	126.024	83.030	42.994	60.132	64491.	-158873.	-23530.	0.819
2 s	----	0.532	0.176	0.478	3.287	717.	714.	139.	0.005

600

Table 8.06. Thermodynamic properties of cuprite and liquid dicuprous oxide, $Cu_2O(s,l)$.

T K	V° cm^3/mol	S°	$\frac{-(G^\circ_T-H^\circ_{298})}{T}$	$\frac{(H^\circ_T-H^\circ_{298})}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
		J/(mol·K)				J/mol			
200.	----	69.149	97.848	-28.700	53.605	-5740.	-170221.	-155209.	40.536
250.	----	81.692	93.390	-11.700	58.775	-2925.	-170453.	-151426.	31.638
2 s	----	0.080	0.091	0.044	0.234	11.	221.	217.	0.045
273.15	----	86.983	92.625	-5.642	60.711	-1541.	-170514.	-149661.	28.619
298.15	----	92.380	92.380	0.000	62.527	0.	-170552.	-147751.	25.885
2 s	----	0.089	0.089	0.000	0.254	0.	226.	216.	0.038
300.	----	92.767	92.382	0.387	62.651	116.	-170554.	-147609.	25.701
350.	----	102.655	93.156	9.500	65.575	3325.	-170559.	-143784.	21.458
400.	----	111.566	94.909	16.658	67.852	6663.	-170492.	-139962.	18.277
450.	----	119.667	97.217	22.451	69.692	10103.	-170370.	-136153.	15.804
500.	----	127.092	99.838	27.254	71.236	13627.	-170203.	-132360.	13.827
2 s	----	0.203	0.101	0.140	0.396	70.	280.	198.	0.021
550.	----	133.946	102.631	31.315	72.579	17223.	-170000.	-128585.	12.212
600.	----	140.314	105.509	34.803	73.783	20882.	-169766.	-124830.	10.867
650.	----	146.264	108.418	37.846	74.892	24600.	-169505.	-121096.	9.731
700.	----	151.852	111.323	40.530	75.936	28371.	-169224.	-117382.	8.759
750.	----	157.126	114.202	42.924	76.937	32193.	-168925.	-113690.	7.918
2 s	----	0.297	0.141	0.184	0.364	138.	342.	153.	0.011
800.	----	162.122	117.042	45.080	77.910	36064.	-168613.	-110017.	7.183
850.	----	166.874	119.835	47.039	78.866	39983.	-168291.	-106365.	6.536
900.	----	171.409	122.575	48.833	79.812	43950.	-167961.	-102732.	5.962
950.	----	175.749	125.261	50.489	80.755	47965.	-167628.	-99117.	5.450
1000.	----	179.916	127.890	52.026	81.699	52026.	-167294.	-95520.	4.989
2 s	----	0.308	0.172	0.193	0.925	193.	367.	112.	0.006
1050.	----	183.925	130.463	53.461	82.646	56134.	-166961.	-91939.	4.574
1100.	----	187.791	132.982	54.810	83.599	60291.	-166633.	-88375.	4.196
1150.	----	191.529	135.446	56.082	84.559	64494.	-166311.	-84825.	3.853
1200.	----	195.148	137.859	57.289	85.528	68747.	-165999.	-81289.	3.538
1250.	----	198.659	140.221	58.438	86.506	73047.	-165697.	-77765.	3.250
2 s	----	0.428	0.186	0.354	1.707	443.	510.	108.	0.005
1300.	----	202.071	142.535	59.536	87.494	77397.	-165409.	-74254.	2.983
1350.	----	205.392	144.801	60.590	88.493	81797.	-165136.	-70753.	2.738
1357.6	----	205.889	145.142	60.747	88.645	82470.	-165096.	-70222.	2.702
2 s	----	0.540	0.192	0.463	2.066	629.	659.	133.	0.005
				Cu(Crystal = Liquid)					
1357.6	----	205.889	145.142	60.747	88.645	82470.	-191343.	-70222.	2.702
1400.	----	208.628	147.023	61.605	89.501	86247.	-191117.	-66442.	2.479
1450.	----	211.787	149.202	62.584	90.520	90747.	-190806.	-61995.	2.233
1500.	----	214.873	151.340	63.533	91.548	95299.	-190447.	-57559.	2.004
2 s	----	0.731	0.208	0.627	2.552	941.	939.	199.	0.007
1516.7	----	215.888	152.045	63.843	91.894	96831.	-190317.	-56080.	1.931
2 s	----	0.756	0.211	0.648	2.610	983.	978.	210.	0.007
				Crystal = Liquid					
1516.7	----	259.143	152.045	107.098	99.614	162435.	-124712.	-56080.	1.931
1550.	----	261.306	154.370	106.937	99.614	165752.	-124190.	-54579.	1.839
1600.	----	264.469	157.761	106.708	99.614	170733.	-123408.	-52346.	1.709
1650.	----	267.534	161.041	106.493	99.614	175713.	-122630.	-50138.	1.587
1700.	----	270.508	164.217	106.291	99.614	180694.	-121853.	-47952.	1.473
1750.	----	273.395	167.296	106.100	99.614	185675.	-121080.	-45790.	1.367
2 s	----	5.209	0.365	4.915	43.987	8601.	8604.	577.	0.017
1800.	----	276.202	170.282	105.919	99.614	190655.	-120308.	-43650.	1.267
2 s	----	6.433	0.495	5.988	43.987	10779.	10782.	846.	0.025

Table 8.07. Thermodynamic properties of alpha and gamma iron, Fe(s1,s2).

T K	V° cm^3/mol	S°	$-(G^\circ_T-H^\circ_{298})/T$	$(H^\circ_T-H^\circ_{298})/T$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
		------------	J/(mol·K)	------------		--------	J/mol	--------	
200.	7.068	17.977	29.510	-11.535	21.688	-2307.	0.	0.	0.000
250.	7.078	23.032	27.721	-4.688	23.589	-1172.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
273.15	7.083	25.154	27.414	-2.259	24.324	-617.	0.	0.	0.000
298.15	7.089	27.316	27.316	0.000	25.054	0.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
300.	7.090	27.471	27.316	0.153	25.106	46.	0.	0.	0.000
350.	7.102	31.441	27.627	3.814	26.398	1335.	0.	0.	0.000
400.	7.116	35.041	28.332	6.708	27.527	2683.	0.	0.	0.000
450.	7.131	38.343	29.263	9.080	28.561	4086.	0.	0.	0.000
500.	7.146	41.405	30.326	11.078	29.568	5539.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
550.	7.162	44.271	31.465	12.805	30.606	7043.	0.	0.	0.000
600.	7.179	46.981	32.646	14.335	31.728	8601.	0.	0.	0.000
650.	7.196	49.569	33.849	15.720	32.983	10218.	0.	0.	0.000
700.	7.214	52.065	35.061	17.003	34.421	11902.	0.	0.	0.000
750.	7.232	54.495	36.276	18.219	36.100	13664.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
800.	7.250	56.887	37.490	19.397	38.099	15518.	0.	0.	0.000
850.	7.268	59.267	38.701	20.567	40.545	17482.	0.	0.	0.000
900.	7.287	61.669	39.910	21.759	43.673	19583.	0.	0.	0.000
950.	7.306	64.140	41.120	23.020	48.029	21869.	0.	0.	0.000
1000.	7.325	66.770	42.336	24.435	55.482	24435.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
1042.00	7.341	69.327	43.370	25.957	72.503	27047.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
---	---	---	---		T_C	---	---	---	---
1042.00	7.341	69.327	43.370	25.957	63.280	27047.	0.	0.	0.000
1050.	7.344	69.786	43.570	26.216	57.300	27527.	0.	0.	0.000
1100.	7.363	72.106	44.816	27.290	45.636	30019.	0.	0.	0.000
1150.	7.382	74.048	46.046	28.003	42.161	32203.	0.	0.	0.000
1184.	7.396	75.257	46.868	28.389	40.859	33613.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
	---	---	---	Fe(alpha) =	Fe(gamma)	---	---	---	---
1184.	7.297	76.016	46.868	29.149	33.862	34512.	0.	0.	0.000
1200.	7.305	76.472	47.259	29.212	33.995	35055.	0.	0.	0.000
1250.	7.331	77.868	48.456	29.412	34.412	36765.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
1300.	7.357	79.226	49.613	29.612	34.828	38496.	0.	0.	0.000
1350.	7.382	80.548	50.735	29.813	35.244	40248.	0.	0.	0.000
1400.	7.408	81.837	51.823	30.015	35.660	42021.	0.	0.	0.000
1450.	7.434	83.096	52.879	30.217	36.077	43814.	0.	0.	0.000
1500.	7.461	84.326	53.907	30.419	36.493	45628.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
1550.	7.487	85.529	54.908	30.621	36.909	47463.	0.	0.	0.000
1600.	7.513	86.708	55.883	30.824	37.326	49319.	0.	0.	0.000
1650.	7.539	87.863	56.835	31.028	37.742	51196.	0.	0.	0.000
1665.	7.547	88.205	57.116	31.089	37.867	51763.	0.	0.	0.000
2 s	0.003	----	----	----	----	----	0.	0.	0.000
	---	---	---	Fe(gamma) =	Fe(alpha)	---	---	---	---
1665.	7.584	88.707	57.116	31.592	41.022	52600.	0.	0.	0.000
1700.	7.598	89.566	57.775	31.791	41.493	54044.	0.	0.	0.000
1750.	7.617	90.779	58.701	32.078	42.212	56136.	0.	0.	0.000
2 s	0.003	----	----	----	----	----	0.	0.	0.000
1800.	7.637	91.978	59.609	32.370	42.981	58266.	0.	0.	0.000
2 s	0.003	----	----	----	----	----	0.	0.	0.000

Table 8.08. Thermodynamic properties of ferrous oxide, FeO(s).

T	V°	S°	$\frac{-(G^\circ_T-H^\circ_{298})}{T}$	$\frac{(H^\circ_T-H^\circ_{298})}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
K	cm³/mol	J/(mol·K)				J/mol			
200.	12.225	45.296	67.659	-22.360	45.317	-4472.	-262831.	-248946.	65.017
250.	12.226	55.227	64.213	-8.984	45.471	-2246.	-262468.	-245518.	51.297
2 s	0.005	0.804	0.693	0.140	0.796	35.	435.	242.	0.051
273.15	12.229	59.307	63.626	-4.320	46.648	-1180.	-262296.	-243956.	46.651
298.15	12.232	63.439	63.439	0.000	47.698	0.	-262100.	-242287.	42.447
2 s	0.004	0.702	0.702	0.000	0.667	0.	409.	208.	0.037
300.	12.233	63.734	63.440	0.293	47.767	88.	-262085.	-242164.	42.164
350.	12.243	71.218	64.027	7.191	49.260	2517.	-261682.	-238875.	35.649
400.	12.256	77.865	65.349	12.515	50.255	5006.	-261288.	-235644.	30.771
450.	12.272	83.827	67.077	16.749	50.962	7537.	-260917.	-232461.	26.983
500.	12.290	89.225	69.026	20.198	51.498	10099.	-260580.	-229318.	23.956
2 s	0.007	0.424	0.638	0.254	0.647	127.	312.	107.	0.011
550.	12.311	94.154	71.090	23.064	51.931	12685.	-260282.	-226207.	21.483
600.	12.333	98.689	73.203	25.485	52.301	15291.	-260031.	-223120.	19.424
650.	12.356	102.889	75.327	27.562	52.633	17915.	-259833.	-220053.	17.683
700.	12.380	106.800	77.437	29.363	52.942	20554.	-259698.	-216998.	16.192
750.	12.406	110.463	79.518	30.945	53.240	23209.	-259634.	-213951.	14.901
2 s	0.007	0.214	0.520	0.364	0.623	273.	192.	44.	0.003
800.	12.432	113.909	81.561	32.348	53.531	25878.	-259657.	-210905.	13.770
839.15	12.453	116.472	83.130	33.341	53.758	27978.	-259747.	-208518.	12.979
2 s	0.007	0.160	0.480	0.381	0.614	320.	153.	35.	0.002
Iron(alpha) - Wustite Solid Solution - Magnetite Coexistance									
839.15	12.453	116.472	83.130	33.341	53.758	27978.	-259747.	-208518.	12.979
850.	12.459	117.163	83.560	33.602	53.821	28562.	-259785.	-207855.	12.773
900.	12.487	120.247	85.513	34.733	54.112	31260.	-260043.	-204794.	11.886
950.	12.515	123.181	87.419	35.761	54.405	33973.	-260478.	-201713.	11.091
1000.	12.544	125.979	89.278	36.701	54.703	36701.	-261185.	-198604.	10.374
2 s	0.006	0.104	0.415	0.394	0.541	394.	111.	29.	0.002
1050.	12.573	128.655	91.090	37.566	55.006	39444.	-262409.	-195446.	9.723
1100.	12.602	131.221	92.856	38.365	55.314	42202.	-263023.	-192241.	9.129
1150.	12.631	133.687	94.578	39.109	55.628	44975.	-263318.	-189016.	8.585
1184.	12.651	135.311	95.724	39.586	55.844	46870.	-263438.	-186818.	8.242
2 s	0.004	0.097	0.351	0.382	0.408	452.	115.	29.	0.001
Fe(alpha) = Fe(gamma)									
1184.	12.651	135.311	95.724	39.586	55.844	46870.	-264338.	-186818.	8.242
1200.	12.661	136.061	96.257	39.803	55.947	47764.	-264271.	-185771.	8.086
1250.	12.691	138.351	97.896	40.456	56.271	50570.	-264071.	-182504.	7.626
2 s	0.004	0.097	0.331	0.370	0.412	462.	119.	31.	0.001
1300.	12.721	140.565	99.494	41.071	56.601	53392.	-263878.	-179245.	7.202
1350.	12.751	142.707	101.055	41.652	56.936	56230.	-263694.	-175994.	6.809
1400.	12.782	144.784	102.580	42.204	57.276	59085.	-263518.	-172749.	6.445
1450.	12.812	146.800	104.070	42.730	57.621	61958.	-263349.	-169510.	6.106
1500.	12.843	148.759	105.528	43.232	57.971	64848.	-263186.	-166277.	5.790
2 s	0.007	0.105	0.272	0.299	0.979	449.	156.	37.	0.001
1550.	12.873	150.666	106.953	43.713	58.325	67755.	-263030.	-163049.	5.495
1600.	12.904	152.523	108.348	44.175	58.684	70680.	-262879.	-159826.	5.218
1650.	12.935	154.335	109.714	44.620	59.046	73623.	-262734.	-156608.	4.958
1665.	12.944	154.870	110.119	44.751	59.156	74510.	-262692.	-155644.	4.883
2 s	0.010	0.195	0.246	0.274	1.645	457.	314.	41.	0.001
Fe(gamma) = Fe(alpha)									
1665.	12.944	154.870	110.119	44.751	59.156	74510.	-263529.	-155644.	4.883
1700.	12.966	156.103	111.053	45.050	59.413	76585.	-263545.	-153376.	4.713
1750.	12.996	157.830	112.365	45.466	59.783	79565.	-263585.	-150135.	4.481
2 s	0.011	0.274	0.238	0.293	2.044	513.	455.	49.	0.001
1800.	13.027	159.520	113.651	45.868	60.157	82563.	-263645.	-146893.	4.263
2 s	0.012	0.330	0.234	0.318	2.294	573.	556.	59.	0.002

Table 8.09. Thermodynamic properties of hematite, Fe_2O_3.

T	V°	S°	$\frac{-(G^\circ_T-H^\circ_{298})}{T}$	$\frac{(H^\circ_T-H^\circ_{298})}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	Δ_fH°	Δ_fG°	$\log {}_fK^\circ$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	30.217	51.555	96.488	-44.935	76.203	-8987.	-824788.	-769862.	201.063
250.	30.244	70.391	89.395	-19.004	92.493	-4751.	-825007.	-756093.	157.974
2 s	0.019	0.202	0.200	0.024	0.114	6.	247.	207.	0.043
273.15	30.258	78.855	88.144	-9.288	98.583	-2537.	-824921.	-749715.	143.365
298.15	30.275	87.740	87.740	0.000	104.274	0.	-824718.	-742840.	130.140
2 s	0.014	0.200	0.200	0.000	0.124	0.	248.	200.	0.035
300.	30.277	88.386	87.742	0.643	104.663	193.	-824699.	-742332.	129.249
350.	30.314	105.235	89.052	16.183	113.747	5664.	-824017.	-728653.	108.743
400.	30.357	120.898	92.065	28.833	120.720	11533.	-823085.	-715091.	93.379
450.	30.402	135.449	96.087	39.362	126.289	17713.	-821984.	-701657.	81.444
500.	30.450	149.002	100.709	48.294	130.945	24147.	-820771.	-688351.	71.910
2 s	0.013	0.208	0.199	0.068	0.197	34.	260.	167.	0.017
550.	30.501	161.678	105.682	55.996	135.039	30798.	-819481.	-675171.	64.121
600.	30.555	173.592	110.849	62.743	138.831	37646.	-818139.	-662111.	57.641
650.	30.610	184.851	116.113	68.738	142.536	44680.	-816765.	-649164.	52.166
700.	30.666	195.552	121.408	74.144	146.352	51901.	-815371.	-636324.	47.482
750.	30.724	205.788	126.694	79.095	150.507	59321.	-813964.	-623584.	43.429
2 s	0.011	0.223	0.199	0.097	0.178	73.	273.	124.	0.009
800.	30.783	215.651	131.947	83.704	155.337	66963.	-812545.	-610938.	39.889
850.	30.842	225.243	137.154	88.089	161.485	74876.	-811101.	-598382.	36.771
900.	30.903	234.710	142.311	92.399	170.582	83159.	-809587.	-585912.	34.005
950.	30.964	244.337	147.426	96.912	188.012	92066.	-807837.	-573531.	31.534
955.53	30.971	245.437	147.990	97.447	191.055	93114.	-807611.	-572168.	31.277
2 s	0.008	0.229	0.199	0.108	0.745	103.	280.	93.	0.005
					T_N				
955.53	30.971	245.437	147.990	97.447	175.199	93114.	-807611.	-572168.	31.277
1000.	31.026	252.647	152.488	100.158	151.106	100158.	-807482.	-561220.	29.314
2 s	0.009	0.231	0.200	0.108	0.462	108.	283.	88.	0.005
1050.	31.088	259.881	157.432	102.449	146.324	107571.	-808878.	-548877.	27.305
1100.	31.151	266.645	162.244	104.401	144.729	114841.	-809233.	-536484.	25.475
1150.	31.214	273.066	166.924	106.142	144.299	122063.	-809033.	-524090.	23.804
1184.	31.257	277.270	170.033	107.237	144.322	126969.	-808761.	-515669.	22.749
2 s	0.015	0.204	0.198	0.112	0.740	133.	258.	77.	0.003
				Fe(alpha) = Fe(gamma)					
1184.	31.257	277.270	170.033	107.237	144.322	126969.	-810560.	-515669.	22.749
1200.	31.277	279.208	171.476	107.732	144.385	129279.	-810192.	-511687.	22.273
1250.	31.341	285.108	175.904	109.205	144.717	136506.	-809069.	-499272.	20.863
2 s	0.018	0.201	0.196	0.132	0.843	165.	257.	77.	0.003
1300.	31.405	290.793	180.214	110.579	145.171	143753.	-807980.	-486902.	19.564
1350.	31.469	296.281	184.412	111.870	145.690	151024.	-806920.	-474573.	18.362
1400.	31.533	301.590	188.502	113.087	146.244	158322.	-805886.	-462283.	17.248
1450.	31.597	306.731	192.491	114.241	146.822	165649.	-804875.	-450029.	16.211
1500.	31.662	311.719	196.382	115.337	147.416	173005.	-803886.	-437810.	15.246
2 s	0.033	0.276	0.186	0.258	1.203	387.	371.	96.	0.003
1550.	31.726	316.562	200.182	116.381	148.023	180391.	-802918.	-425623.	14.343
1600.	31.791	321.272	203.892	117.379	148.643	187807.	-801970.	-413468.	13.498
1650.	31.855	325.855	207.519	118.336	149.275	195255.	-801041.	-401341.	12.705
1665.	31.874	327.207	208.591	118.616	149.466	197496.	-800766.	-397709.	12.477
2 s	0.043	0.382	0.180	0.358	1.442	596.	547.	131.	0.004
				Fe(gamma) = Fe(alpha)					
1665.	31.874	327.207	208.591	118.616	149.466	197496.	-802439.	-397709.	12.477
1700.	31.920	330.321	211.065	119.256	149.917	202735.	-802030.	-389206.	11.959
1750.	31.984	334.676	214.535	120.141	150.572	210247.	-801484.	-377072.	11.255
2 s	0.049	0.446	0.178	0.412	1.567	721.	662.	158.	0.005
1800.	32.049	338.927	217.932	120.996	151.237	217792.	-800986.	-364953.	10.590
2 s	0.052	0.486	0.179	0.444	1.640	799.	736.	177.	0.005

Table 8.10. Thermodynamic properties of fayalite and liquid diferrous silicate, Fe_2SiO_4(sl,l).

T	V°	S°	$-(G^\circ_T-H^\circ_{298})/T$	$(H^\circ_T-H^\circ_{298})/T$	C°_P	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log $_f K^\circ$
K	cm³/mol	J/(mol·K)				J/mol			
200.	46.068	104.144	162.160	-58.015	101.983	-11603.	-1477261.	-1411174.	368.553
250.	46.117	128.817	153.052	-24.236	119.116	-6059.	-1477752.	-1394586.	291.377
2 s	0.024	1.017	1.017	0.040	0.215	10.	1331.	1122.	0.234
273.15	46.141	139.660	151.460	-11.799	125.714	-3223.	-1477816.	-1386881.	265.208
298.15	46.169	150.947	150.947	0.000	132.017	0.	-1477783.	-1378559.	241.513
2 s	0.024	1.017	1.017	0.000	0.221	0.	1331.	1083.	0.190
300.	46.171	151.765	150.950	0.817	132.452	245.	-1477777.	-1377943.	239.916
350.	46.230	172.995	152.602	20.391	142.840	7137.	-1477442.	-1361326.	203.163
400.	46.293	192.625	156.394	36.230	151.049	14492.	-1476856.	-1344776.	175.606
450.	46.359	210.811	161.443	49.369	157.642	22216.	-1476097.	-1328310.	154.183
500.	46.428	227.708	167.235	60.472	163.016	30236.	-1475227.	-1311935.	137.054
2 s	0.024	1.027	1.016	0.148	0.688	74.	1347.	932.	0.097
550.	46.499	243.459	173.456	70.004	167.455	38502.	-1474293.	-1295651.	123.048
600.	46.572	258.193	179.911	78.283	171.162	46970.	-1473337.	-1279453.	111.384
650.	46.647	272.021	186.470	85.551	174.288	55608.	-1472397.	-1263334.	101.521
700.	46.724	285.037	193.050	91.987	176.945	64391.	-1471508.	-1247286.	93.072
750.	46.801	297.324	199.596	97.728	179.220	73296.	-1470707.	-1231299.	85.753
2 s	0.024	1.118	1.020	0.385	1.099	289.	1424.	754.	0.053
800.	46.880	308.955	206.070	102.884	181.177	82307.	-1470034.	-1215361.	79.353
850.	46.960	319.991	212.450	107.541	182.870	91410.	-1469538.	-1199461.	73.708
900.	47.040	330.486	218.718	111.768	184.339	100591.	-1469281.	-1183583.	68.692
950.	47.120	340.487	224.866	115.621	185.618	109840.	-1469361.	-1167710.	64.204
1000.	47.202	350.037	230.888	119.150	186.733	119150.	-1469980.	-1151821.	60.164
2 s	0.024	1.238	1.036	0.535	1.795	535.	1535.	619.	0.032
1050.	47.284	359.172	236.780	122.391	187.708	128511.	-1471632.	-1135876.	56.506
1100.	47.366	367.924	242.544	125.381	188.560	137919.	-1472068.	-1119873.	53.177
1150.	47.448	376.323	248.179	128.144	189.305	147366.	-1471876.	-1103868.	50.138
1184.	47.505	381.846	251.939	129.907	189.757	153810.	-1471590.	-1092991.	48.219
2 s	0.024	1.357	1.053	0.697	3.227	825.	1665.	594.	0.026
				Fe(alpha) = Fe(gamma)					
1184.	47.505	381.846	251.939	129.907	189.757	153810.	-1473390.	-1092991.	48.219
1200.	47.531	384.394	253.688	130.706	189.956	156847.	-1473013.	-1087853.	47.352
1250.	47.614	392.160	259.072	133.088	190.523	166360.	-1471861.	-1071829.	44.788
2 s	0.025	1.430	1.060	0.798	3.893	997.	1752.	609.	0.025
1300.	47.697	399.642	264.336	135.307	191.016	175899.	-1470747.	-1055850.	42.424
1350.	47.781	406.860	269.482	137.378	191.443	185460.	-1469674.	-1039912.	40.236
1400.	47.864	413.829	274.513	139.316	191.811	195042.	-1468644.	-1024014.	38.206
1450.	47.948	420.565	279.434	141.132	192.126	204641.	-1467657.	-1008152.	36.317
1490.	48.015	425.797	283.293	142.503	192.343	212330.	-1466901.	-995487.	34.898
2 s	0.025	1.953	1.095	1.397	6.808	2082.	2494.	790.	0.028
				Crystal = Liquid					
1490.	50.798	484.890	283.293	201.597	226.834	300379.	-1378852.	-995487.	34.898
1500.	50.798	486.407	284.642	201.765	226.834	302647.	-1378323.	-992915.	34.576
2 s	0.661	2.486	1.097	2.065	2.082	3098.	3390.	803.	0.028
1550.	50.798	493.845	291.271	202.574	226.834	313989.	-1375714.	-980112.	33.029
1600.	50.798	501.047	297.715	203.332	226.834	325331.	-1373163.	-967391.	31.581
1650.	50.798	508.027	303.983	204.044	226.834	336672.	-1370670.	-954750.	30.224
1665.	50.798	510.080	305.830	204.249	226.834	340075.	-1369933.	-950972.	29.833
2 s	0.661	2.499	1.147	1.876	2.082	3123.	3413.	1072.	0.034
				Fe(gamma) = Fe(alpha)					
1665.	50.798	510.080	305.830	204.249	226.834	340075.	-1371607.	-950972.	29.833
1685.	50.798	512.788	308.271	204.518	226.834	344612.	-1370761.	-945924.	29.323
2 s	0.661	2.501	1.154	1.857	2.082	3129.	3418.	1111.	0.034
				Si(Crystal = Liquid)					
1685.	50.798	512.788	308.271	204.518	226.834	344612.	-1421312.	-945924.	29.323
1700.	50.798	514.798	310.084	204.714	226.834	348014.	-1420644.	-941695.	28.934
1750.	50.798	521.374	316.028	205.346	226.834	359356.	-1418471.	-927640.	27.688
2 s	0.661	2.511	1.180	1.801	2.082	3151.	3438.	1242.	0.037
1800.	50.798	527.764	321.821	205.943	226.834	370698.	-1416383.	-913646.	26.513
2 s	0.661	2.520	1.201	1.762	2.082	3171.	3457.	1348.	0.039

Table 8.11. Thermodynamic properties of diferrous silicate (spinel structure), Fe_2SiO_4(s2).

T K	V° cm^3/mol	S°	$-(G^\circ_T - H^\circ_{298})/T$	$(H^\circ_T - H^\circ_{298})/T$	C°_p	$H^\circ_T - H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
		-------------J/(mol·K)	------------			--------J/mol	--------		
200.	41.901	92.273	150.932	-58.660	103.685	-11732.	-1470624.	-1402163.	366.200
250.	41.996	117.358	141.739	-24.380	120.613	-6095.	-1471023.	-1384992.	289.372
2 s	0.061	3.712	3.656	0.684	4.930	171.	3399.	2576.	0.538
273.15	42.036	128.304	140.140	-11.836	126.519	-3233.	-1471060.	-1377023.	263.323
298.15	42.076	139.626	139.626	0.000	131.979	0.	-1471017.	-1368418.	239.736
2 s	0.049	3.656	3.656	0.000	2.557	0.	3399.	2426.	0.425
300.	42.079	140.443	139.628	0.817	132.351	245.	-1471011.	-1367781.	238.147
350.	42.151	161.533	141.274	20.260	141.113	7091.	-1470723.	-1350596.	201.561
400.	42.215	180.842	145.030	35.813	147.985	14325.	-1470258.	-1333465.	174.129
450.	42.270	198.605	150.009	48.596	153.568	21868.	-1469679.	-1316399.	152.800
500.	42.320	215.033	155.701	59.332	158.226	29666.	-1469031.	-1299402.	135.745
2 s	0.054	3.478	3.616	0.662	1.987	331.	3361.	1838.	0.192
550.	42.364	230.304	161.797	68.507	162.193	37679.	-1468350.	-1282472.	121.797
600.	42.403	244.567	168.106	76.460	165.628	45876.	-1467665.	-1265605.	110.178
650.	42.439	257.946	174.508	83.438	168.642	54235.	-1467005.	-1248793.	100.352
700.	42.471	270.544	180.922	89.621	171.318	62735.	-1466398.	-1232031.	91.933
750.	42.501	282.447	187.297	95.149	173.715	71362.	-1465875.	-1215310.	84.640
2 s	0.070	3.054	3.472	1.067	3.261	800.	3144.	1302.	0.091
800.	42.528	293.728	193.600	100.129	175.880	80103.	-1465473.	-1198619.	78.260
850.	42.554	304.451	199.808	104.644	177.849	88947.	-1465235.	-1181949.	72.632
900.	42.577	314.668	205.907	108.761	179.652	97885.	-1465221.	-1165287.	67.630
950.	42.600	324.426	211.890	112.536	181.311	106909.	-1465527.	-1148617.	63.154
1000.	42.621	333.766	217.752	116.014	182.846	116014.	-1466350.	-1131920.	59.124
2 s	0.154	2.731	3.258	1.718	6.092	1718.	2904.	1127.	0.059
1050.	42.641	342.722	223.491	119.230	184.271	125192.	-1468185.	-1115157.	55.475
1100.	42.660	351.325	229.108	122.217	185.600	134439.	-1468781.	-1098328.	52.154
1150.	42.678	359.603	234.603	125.001	186.844	143751.	-1468725.	-1081489.	49.122
1184.	42.690	365.059	238.271	126.788	187.646	150117.	-1468517.	-1070043.	47.206
2 s	0.239	2.961	3.083	2.466	8.563	2920.	3170.	1258.	0.056
				Fe(alpha) = Fe(gamma)					
1184.	42.690	365.059	238.271	126.788	187.646	150117.	-1470316.	-1070043.	47.206
1200.	42.696	367.580	239.978	127.602	188.012	153123.	-1469972.	-1064636.	46.341
1250.	42.713	375.278	245.237	130.041	189.112	162551.	-1468904.	-1047769.	43.783
2 s	0.271	3.182	3.023	2.778	9.486	3473.	3451.	1357.	0.057
1300.	42.730	382.715	250.382	132.333	190.150	172033.	-1467847.	-1030944.	41.423
1350.	42.747	389.910	255.418	134.493	191.133	181565.	-1466804.	-1014160.	39.239
1400.	42.763	396.878	260.346	136.532	192.065	191145.	-1465775.	-997415.	37.213
1450.	42.779	403.634	265.171	138.463	192.952	200771.	-1464761.	-980705.	35.328
1500.	42.794	410.189	269.896	140.293	193.796	210440.	-1463765.	-964031.	33.570
2 s	0.401	4.577	2.844	4.107	13.083	6160.	5503.	1995.	0.069
1550.	42.810	416.557	274.525	142.032	194.603	220150.	-1462787.	-947389.	31.926
1600.	42.825	422.748	279.061	143.687	195.373	229899.	-1461829.	-930779.	30.386
1650.	42.840	428.771	283.507	145.265	196.112	239687.	-1460890.	-914198.	28.940
1665.	42.845	430.547	284.823	145.724	196.327	242630.	-1460613.	-909229.	28.524
2 s	0.490	5.834	2.806	5.076	15.510	8451.	7601.	2683.	0.084
				Fe(gamma) = Fe(alpha)					
1665.	42.845	430.547	284.823	145.724	196.327	242630.	-1462286.	-909229.	28.524
1685.	42.851	432.893	286.567	146.326	196.610	246559.	-1462047.	-902587.	27.979
2 s	0.501	5.999	2.808	5.197	15.806	8757.	7890.	2783.	0.086
				Si(Crystal = Liquid)					
1685.	42.851	432.893	286.567	146.326	196.610	246559.	-1512598.	-902587.	27.979
1700.	42.855	434.636	287.866	146.771	196.820	249510.	-1512382.	-897158.	27.566
1750.	42.870	440.351	292.141	148.210	197.500	259368.	-1511693.	-879073.	26.238
2 s	0.536	6.551	2.824	5.595	16.770	9792.	8880.	3133.	0.094
1800.	42.885	445.924	296.336	149.588	198.154	269259.	-1511055.	-861008.	24.985
2 s	0.564	6.991	2.847	5.907	17.514	10633.	9691.	3430.	0.100

Table 8.12. Thermodynamic properties of magnetite, Fe_3O_4(s).

T K	V° cm^3/mol	S°	$-(G^\circ_T-H^\circ_{298})/T$	$(H^\circ_T-H^\circ_{298})/T$	C°_P	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log $_fK^\circ$
		-------------	J/(mol·K)	-----------		--------	J/mol	--------	
200.	44.454	92.700	158.931	-66.230	116.845	-13246.	-1116714.	-1047073.	273.462
250.	44.491	120.900	148.539	-27.640	135.874	-6910.	-1116696.	-1029652.	215.129
2 s	0.011	0.070	0.038	0.064	0.461	16.	90.	86.	0.018
273.15	44.514	133.264	146.723	-13.458	143.349	-3676.	-1116483.	-1021600.	195.357
298.15	44.542	146.138	146.138	0.000	150.626	0.	-1116125.	-1012931.	177.458
2 s	0.012	0.038	0.038	0.000	0.280	0.	88.	85.	0.015
300.	44.544	147.071	146.141	0.930	151.134	279.	-1116094.	-1012291.	176.252
350.	44.610	171.329	148.028	23.300	163.484	8155.	-1115033.	-995069.	148.503
400.	44.687	193.844	152.365	41.480	173.681	16592.	-1113628.	-978023.	127.714
450.	44.773	214.818	158.153	56.664	182.447	25499.	-1111961.	-961171.	111.567
500.	44.867	234.458	164.811	69.646	190.428	34823.	-1110081.	-944515.	98.671
2 s	0.015	0.147	0.047	0.116	0.449	58.	143.	74.	0.008
550.	44.968	252.972	171.992	80.980	198.207	44539.	-1108015.	-928057.	88.138
600.	45.074	270.563	179.479	91.083	206.352	54650.	-1105765.	-911795.	79.377
650.	45.185	287.432	187.138	100.294	215.509	65191.	-1103310.	-895729.	71.980
700.	45.301	303.793	194.889	108.904	226.611	76233.	-1100599.	-879861.	65.655
750.	45.419	319.905	202.687	117.217	241.494	87913.	-1097522.	-864199.	60.187
2 s	0.013	0.251	0.090	0.176	0.571	132.	210.	25.	0.002
800.	45.541	336.178	210.519	125.660	265.535	100528.	-1093823.	-848760.	55.417
849.1	45.663	353.376	218.271	135.104	292.220	114717.	-1088744.	-833860.	51.296
2 s	0.012	0.267	0.105	0.197	2.616	167.	224.	12.	0.001
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849.1	45.663	353.376	218.271	135.104	292.220	114717.	-1088744.	-833860.	51.296
850.	45.665	353.682	218.414	135.268	287.211	114978.	-1088654.	-833589.	51.225
900.	45.791	367.440	226.330	141.110	221.122	126999.	-1086357.	-818668.	47.513
950.	45.919	379.035	234.067	144.967	209.722	137719.	-1085942.	-803813.	44.196
1000.	46.048	389.672	241.585	148.087	205.660	148087.	-1086746.	-788949.	41.210
2 s	0.016	0.236	0.121	0.149	0.697	149.	197.	42.	0.002
1050.	46.179	399.665	248.876	150.789	204.251	158328.	-1089282.	-774004.	38.504
1100.	46.311	409.157	255.948	153.209	203.953	168530.	-1090075.	-758965.	36.040
1150.	46.443	418.227	262.808	155.419	204.151	178732.	-1089966.	-743916.	33.789
1184.	46.534	424.179	267.357	156.822	204.428	185677.	-1089669.	-733689.	32.368
2 s	0.024	0.215	0.129	0.158	1.014	187.	195.	79.	0.003
- - - - -	- - - - -	- - - - -	- - - - -	Fe(alpha) =	Fe(gamma)	- - - - -	- - - - -	- - - - -	- - - - -
1184.	46.534	424.179	267.357	156.822	204.428	185677.	-1092368.	-733689.	32.368
1200.	46.576	426.924	269.466	157.457	204.583	188949.	-1091865.	-728845.	31.725
1250.	46.710	435.286	275.933	159.354	205.136	199192.	-1090331.	-713751.	29.825
2 s	0.028	0.227	0.130	0.186	1.123	233.	225.	90.	0.004
1300.	46.845	443.344	282.218	161.126	205.759	209464.	-1088847.	-698717.	28.074
1350.	46.980	451.122	288.330	162.792	206.430	219769.	-1087408.	-683740.	26.455
1400.	47.115	458.642	294.279	164.363	207.141	230108.	-1086011.	-668815.	24.953
1450.	47.251	465.924	300.073	165.850	207.888	240483.	-1084654.	-653939.	23.557
1500.	47.387	472.984	305.720	167.265	208.671	250897.	-1083335.	-639109.	22.255
2 s	0.043	0.366	0.128	0.342	1.500	513.	476.	136.	0.005
1550.	47.524	479.840	311.226	168.614	209.488	261351.	-1082050.	-624323.	21.039
1600.	47.660	486.504	316.600	169.904	210.342	271847.	-1080798.	-609577.	19.900
1650.	47.797	492.990	321.847	171.143	211.231	282386.	-1079576.	-594871.	18.832
1665.	47.838	494.903	323.398	171.505	211.505	285556.	-1079215.	-590466.	18.524
2 s	0.054	0.501	0.132	0.455	1.715	757.	714.	184.	0.006
- - - - -	- - - - -	- - - - -	- - - - -	Fe(gamma) =	Fe(alpha)	- - - - -	- - - - -	- - - - -	- - - - -
1665.	47.838	494.903	323.398	171.505	211.505	285556.	-1081725.	-590466.	18.524
1700.	47.933	499.310	326.974	172.335	212.158	292970.	-1081232.	-580144.	17.825
1750.	48.070	505.474	331.987	173.487	213.121	303602.	-1080586.	-565416.	16.876
2 s	0.060	0.576	0.139	0.511	1.821	895.	851.	218.	0.007
1800.	48.207	511.491	336.890	174.602	214.122	314283.	-1080012.	-550705.	15.981
2 s	0.064	0.621	0.145	0.544	1.884	980.	936.	242.	0.007

Table 8.13. Thermodynamic properties of hydrogen, $H_2(g)$.

T	V°	S°	$\frac{-(G^\circ_T-H^\circ_{298})}{T}$	$\frac{(H^\circ_T-H^\circ_{298})}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
K	cm^3/mol	J/(mol·K)				J/mol			
200.	----	119.412	133.284	-13.870	27.556	-2774.	0.	0.	0.000
250.	----	125.644	131.153	-5.508	28.324	-1377.	0.	0.	0.000
273.15	----	128.165	130.794	-2.629	28.607	-718.	0.	0.	0.000
298.15	----	130.680	130.680	0.000	28.832	0.	0.	0.	0.000
300.	----	130.859	130.681	0.177	28.846	53.	0.	0.	0.000
350.	----	135.327	131.033	4.294	29.096	1503.	0.	0.	0.000
400.	----	139.220	131.818	7.400	29.195	2960.	0.	0.	0.000
450.	----	142.661	132.836	9.824	29.229	4421.	0.	0.	0.000
500.	----	145.741	133.975	11.766	29.243	5883.	0.	0.	0.000
550.	----	148.529	135.173	13.356	29.262	7346.	0.	0.	0.000
600.	----	151.076	136.394	14.683	29.296	8810.	0.	0.	0.000
650.	----	153.423	137.615	15.809	29.350	10276.	0.	0.	0.000
700.	----	155.601	138.823	16.779	29.425	11745.	0.	0.	0.000
750.	----	157.634	140.010	17.624	29.520	13218.	0.	0.	0.000
800.	----	159.543	141.172	18.371	29.633	14697.	0.	0.	0.000
850.	----	161.343	142.306	19.038	29.763	16182.	0.	0.	0.000
900.	----	163.049	143.411	19.638	29.907	17674.	0.	0.	0.000
950.	----	164.670	144.488	20.182	30.065	19173.	0.	0.	0.000
1000.	----	166.216	145.536	20.680	30.233	20680.	0.	0.	0.000
1050.	----	167.695	146.556	21.139	30.411	22196.	0.	0.	0.000
1100.	----	169.114	147.549	21.565	30.598	23722.	0.	0.	0.000
1150.	----	170.479	148.517	21.962	30.792	25256.	0.	0.	0.000
1200.	----	171.794	149.459	22.334	30.992	26801.	0.	0.	0.000
1250.	----	173.063	150.378	22.685	31.197	28356.	0.	0.	0.000
1300.	----	174.290	151.275	23.016	31.407	29921.	0.	0.	0.000
1350.	----	175.480	152.149	23.330	31.621	31496.	0.	0.	0.000
1400.	----	176.634	153.003	23.631	31.838	33083.	0.	0.	0.000
1450.	----	177.755	153.837	23.917	32.058	34680.	0.	0.	0.000
1500.	----	178.845	154.653	24.193	32.281	36289.	0.	0.	0.000
1550.	----	179.907	155.450	24.457	32.505	37908.	0.	0.	0.000
1600.	----	180.943	156.231	24.712	32.731	39539.	0.	0.	0.000
1650.	----	181.954	156.995	24.958	32.959	41181.	0.	0.	0.000
1700.	----	182.941	157.744	25.197	33.188	42835.	0.	0.	0.000
1750.	----	183.906	158.478	25.429	33.417	44500.	0.	0.	0.000
1800.	----	184.851	159.197	25.654	33.648	46177.	0.	0.	0.000

Table 8.14. Thermodynamic properties of ice, water, and ideal gas, $H_2O(s,l,g)$.

T	V°	S°	$\frac{-(G^\circ_T-H^\circ_{298})}{T}$	$\frac{(H^\circ_T-H^\circ_{298})}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
K	cm^3/mol	-------------J/(mol·K)------------				--------J/mol--------			
200.	----	31.140	82.679	-51.540	28.139	-10308.	-291881.	-254877.	66.566
250.	----	38.123	73.071	-34.948	34.713	-8737.	-292436.	-245557.	51.305
273.15	----	41.330	70.245	-28.915	37.756	-7898.	-292595.	-241208.	46.125
				Ice = Water					
273.15	----	63.329	70.245	-6.916	75.887	-1889.	-286586.	-241208.	46.125
298.15	----	69.947	69.947	0.000	75.345	0.	-285782.	-237091.	41.536
300.	----	70.413	69.948	0.463	75.327	139.	-285723.	-236789.	41.228
350.	----	82.026	70.865	11.163	75.550	3907.	-284142.	-228758.	34.140
372.78	----	86.802	71.694	15.108	75.932	5632.	-283419.	-225176.	31.551
				Water = Gas					
372.78	----	196.381	71.706	124.674	34.000	46476.	-242575.	-225181.	31.552
400.	----	198.784	80.273	118.510	34.202	47404.	-242849.	-223901.	29.238
450.	----	202.837	93.670	109.167	34.650	49125.	-243347.	-221502.	25.711
500.	----	206.515	104.773	101.742	35.175	50871.	-243834.	-219049.	22.883
550.	----	209.894	114.178	95.716	35.754	52644.	-244308.	-216547.	20.566
600.	----	213.031	122.286	90.745	36.368	54447.	-244766.	-214003.	18.630
650.	----	215.967	129.381	86.586	37.004	56281.	-245207.	-211422.	16.990
700.	----	218.733	135.665	83.067	37.652	58147.	-245629.	-208807.	15.581
750.	----	221.353	141.291	80.061	38.306	60046.	-246033.	-206163.	14.358
800.	----	223.846	146.374	77.473	38.959	61978.	-246419.	-203492.	13.286
850.	----	226.227	151.001	75.226	39.608	63942.	-246787.	-200798.	12.339
900.	----	228.509	155.244	73.266	40.252	65939.	-247137.	-198082.	11.496
950.	----	230.703	159.159	71.544	40.887	67967.	-247470.	-195348.	10.741
1000.	----	232.816	162.789	70.027	41.514	70027.	-247786.	-192596.	10.060
1050.	----	234.857	166.172	68.684	42.130	72118.	-248085.	-189829.	9.443
1100.	----	236.830	169.340	67.491	42.737	74240.	-248369.	-187049.	8.882
1150.	----	238.743	172.316	66.428	43.333	76392.	-248637.	-184255.	8.369
1200.	----	240.600	175.122	65.477	43.918	78573.	-248890.	-181451.	7.898
1250.	----	242.405	177.778	64.626	44.493	80783.	-249129.	-178636.	7.465
1300.	----	244.161	180.297	63.863	45.058	83022.	-249354.	-175811.	7.064
1350.	----	245.872	182.694	63.177	45.613	85289.	-249566.	-172979.	6.693
1400.	----	247.540	184.981	62.559	46.158	87583.	-249764.	-170139.	6.348
1450.	----	249.169	187.166	62.003	46.693	89905.	-249950.	-167292.	6.026
1500.	----	250.761	189.260	61.502	47.219	92253.	-250123.	-164438.	5.726
1550.	----	252.318	191.269	61.049	47.736	94626.	-250285.	-161579.	5.445
1600.	----	253.842	193.200	60.641	48.245	97026.	-250435.	-158715.	5.181
1650.	----	255.334	195.061	60.273	48.745	99451.	-250575.	-155847.	4.934
1700.	----	256.796	196.855	59.941	49.237	101900.	-250703.	-152975.	4.700
1750.	----	258.231	198.588	59.642	49.721	104374.	-250821.	-150098.	4.480
1800.	----	259.638	200.264	59.373	50.198	106872.	-250929.	-147219.	4.272

Note: The Gibbs energy of formation and related functions are not identical at the 1-bar boiling temperature because the vapor phase is not an ideal gas. The temperature at which water and steam have identical Gibbs energies at 1 bar is approximately 373.19 K.

Table 8.15. Thermodynamic properties of steam, $H_2(g)$.

T K	V° cm^3/mol	S°	$-(G^\circ_T-H^\circ_{298})/T$	$(H^\circ_T-H^\circ_{298})/T$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
		-------------J/(mol·K)------------				--------J/mol--------			
200.	----	175.524	191.895	-16.370	32.830	-3274.	-240892.	-232766.	60.791
250.	----	182.931	189.387	-6.456	33.422	-1614.	-241358.	-230681.	48.197
273.15	----	185.895	188.967	-3.072	33.522	-839.	-241581.	-229682.	43.921
298.15	----	188.835	188.835	0.000	33.613	0.	-241827.	-228582.	40.046
300.	----	189.043	188.835	0.207	33.620	62.	-241845.	-228500.	39.785
350.	----	194.242	189.245	4.997	33.856	1749.	-242345.	-226237.	33.763
400.	----	198.784	190.160	8.625	34.202	3450.	-242849.	-223901.	29.238
450.	----	202.837	191.347	11.491	34.650	5171.	-243347.	-221502.	25.711
500.	----	206.515	192.683	13.832	35.175	6916.	-243834.	-219049.	22.883
550.	----	209.894	194.096	15.798	35.754	8689.	-244308.	-216547.	20.566
600.	----	213.031	195.544	17.487	36.368	10492.	-244766.	-214003.	18.630
650.	----	215.967	197.004	18.963	37.004	12326.	-245207.	-211422.	16.990
700.	----	218.733	198.458	20.274	37.652	14192.	-245629.	-208807.	15.581
750.	----	221.353	199.898	21.455	38.306	16091.	-246033.	-206163.	14.358
800.	----	223.846	201.317	22.529	38.959	18023.	-246419.	-203492.	13.286
850.	----	226.227	202.713	23.514	39.608	19987.	-246787.	-200798.	12.339
900.	----	228.509	204.083	24.427	40.252	21984.	-247137.	-198082.	11.496
950.	----	230.703	205.427	25.276	40.887	24012.	-247470.	-195348.	10.741
1000.	----	232.816	206.744	26.072	41.514	26072.	-247786.	-192596.	10.060
1050.	----	234.857	208.034	26.822	42.130	28163.	-248085.	-189829.	9.443
1100.	----	236.830	209.298	27.532	42.737	30285.	-248369.	-187049.	8.882
1150.	----	238.743	210.537	28.206	43.333	32437.	-248637.	-184255.	8.369
1200.	----	240.600	211.751	28.848	43.918	34618.	-248890.	-181451.	7.898
1250.	----	242.405	212.942	29.463	44.493	36829.	-249129.	-178636.	7.465
1300.	----	244.161	214.109	30.052	45.058	39067.	-249354.	-175811.	7.064
1350.	----	245.872	215.254	30.618	45.613	41334.	-249566.	-172979.	6.693
1400.	----	247.540	216.377	31.164	46.158	43629.	-249764.	-170139.	6.348
1450.	----	249.169	217.480	31.690	46.693	45950.	-249950.	-167292.	6.026
1500.	----	250.761	218.563	32.199	47.219	48298.	-250123.	-164438.	5.726
1550.	----	252.318	219.627	32.692	47.736	50672.	-250285.	-161579.	5.445
1600.	----	253.842	220.672	33.169	48.245	53071.	-250435.	-158715.	5.181
1650.	----	255.334	221.700	33.634	48.745	55496.	-250575.	-155847.	4.934
1700.	----	256.796	222.711	34.086	49.237	57946.	-250703.	-152975.	4.700
1750.	----	258.231	223.705	34.526	49.721	60420.	-250821.	-150098.	4.480
1800.	----	259.638	224.684	34.954	50.198	62918.	-250929.	-147219.	4.272

Table 8.16. Thermodynamic properties of nickel, Ni(s,l).

T	$V°$	$S°$	$\frac{-(G°_T-H°_{298})}{T}$	$\frac{(H°_T-H°_{298})}{T}$	$C°_P$	$H°_T-H°_{298}$	$\Delta_f H°$	$\Delta_f G°$	$\log {}_f K°$
K	cm^3/mol	J/(mol·K)				J/mol			
200.	6.533	20.238	32.225	-11.985	22.428	-2397.	0.	0.	0.000
250.	6.544	25.484	30.364	-4.880	24.552	-1220.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
273.15	6.550	27.693	30.045	-2.350	25.322	-642.	0.	0.	0.000
298.15	6.556	29.943	29.943	0.000	26.044	0.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
300.	6.556	30.104	29.943	0.160	26.093	48.	0.	0.	0.000
350.	6.569	34.220	30.266	3.954	27.300	1384.	0.	0.	0.000
400.	6.583	37.935	30.996	6.940	28.358	2776.	0.	0.	0.000
450.	6.598	41.335	31.958	9.378	29.400	4220.	0.	0.	0.000
500.	6.613	44.491	33.055	11.436	30.553	5718.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
550.	6.628	47.468	34.231	13.236	32.017	7280.	0.	0.	0.000
600.	6.644	50.346	35.455	14.892	34.495	8935.	0.	0.	0.000
631.	6.654	52.173	36.231	15.943	35.194	10060.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
					T_N				
631.	6.654	52.173	36.231	15.943	35.194	10060.	0.	0.	0.000
650.	6.660	53.170	36.711	16.458	32.668	10698.	0.	0.	0.000
700.	6.676	55.533	37.973	17.560	31.436	12292.	0.	0.	0.000
750.	6.693	57.691	39.216	18.475	31.179	13856.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
800.	6.710	59.702	40.435	19.268	31.189	15414.	0.	0.	0.000
850.	6.727	61.597	41.624	19.973	31.331	16977.	0.	0.	0.000
900.	6.744	63.394	42.784	20.610	31.554	18549.	0.	0.	0.000
950.	6.761	65.107	43.914	21.193	31.831	20133.	0.	0.	0.000
1000.	6.779	66.748	45.015	21.732	32.147	21732.	0.	0.	0.000
2 s	0.001	----	----	----	----	----	0.	0.	0.000
1050.	6.796	68.324	46.088	22.236	32.495	23348.	0.	0.	0.000
1100.	6.814	69.844	47.133	22.711	32.867	24982.	0.	0.	0.000
1150.	6.831	71.314	48.153	23.161	33.259	26635.	0.	0.	0.000
1200.	6.849	72.738	49.148	23.590	33.669	28308.	0.	0.	0.000
1250.	6.867	74.121	50.119	24.002	34.094	30002.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
1300.	6.884	75.467	51.068	24.398	34.532	31718.	0.	0.	0.000
1350.	6.902	76.779	51.996	24.782	34.982	33456.	0.	0.	0.000
1400.	6.920	78.059	52.904	25.155	35.444	35217.	0.	0.	0.000
1450.	6.938	79.311	53.793	25.517	35.915	37000.	0.	0.	0.000
1500.	6.956	80.537	54.665	25.872	36.395	38808.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
1550.	6.974	81.738	55.519	26.219	36.884	40640.	0.	0.	0.000
1600.	6.991	82.917	56.356	26.561	37.381	42497.	0.	0.	0.000
1650.	7.009	84.075	57.179	26.896	37.885	44378.	0.	0.	0.000
1700.	7.027	85.213	57.987	27.226	38.396	46285.	0.	0.	0.000
1728.	7.037	85.843	58.433	27.410	38.685	47364.	0.	0.	0.000
2 s	0.002	----	----	----	----	----	0.	0.	0.000
				Crystal = Liquid					
1728.	7.433	95.770	58.433	37.337	38.952	64519.	0.	0.	0.000
1750.	7.455	96.263	58.905	37.358	38.952	65376.	0.	0.	0.000
2 s	1.448	----	----	----	----	----	0.	0.	0.000
1800.	7.506	97.360	59.959	37.402	38.952	67323.	0.	0.	0.000
2 s	1.298	----	----	----	----	----	0.	0.	0.000

Table 8.17. Thermodynamic properties of bunsenite, NiO(s).

T	V°	S°	$\frac{-(G^\circ_T-H^\circ_{298})}{T}$	$\frac{(H^\circ_T-H^\circ_{298})}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log_f K^\circ$
K	cm^3/mol	------------J/(mol·K)------------				--------J/mol--------			
200.	10.949	22.355	41.602	-19.245	34.267	-3849.	-239004.	-220079.	57.477
250.	10.968	30.507	38.579	-8.072	39.288	-2018.	-239079.	-215336.	44.991
2 s	0.015	0.113	0.107	0.036	0.191	9.	146.	126.	0.026
273.15	10.976	34.098	38.048	-3.950	41.837	-1079.	-239056.	-213138.	40.758
298.15	10.986	37.876	37.876	0.000	44.450	0.	-238986.	-210768.	36.925
2 s	0.016	0.107	0.107	0.000	0.168	0.	146.	122.	0.021
300.	10.987	38.151	37.876	0.273	44.636	82.	-238979.	-210593.	36.667
350.	11.008	45.389	38.437	6.951	49.275	2433.	-238702.	-205882.	30.726
400.	11.029	52.241	39.739	12.502	53.398	5001.	-238272.	-201221.	26.276
450.	11.051	58.770	41.493	17.278	57.648	7775.	-237701.	-196623.	22.823
500.	11.073	65.138	43.539	21.598	64.167	10799.	-236945.	-192097.	20.068
2 s	0.016	0.122	0.108	0.044	0.202	22.	153.	106.	0.011
519.	11.082	67.616	44.375	23.241	69.259	12062.	-236564.	-190399.	19.162
2 s	0.016	0.123	0.109	0.044	0.335	23.	153.	105.	0.011
					T_N				
519.	11.082	67.616	44.375	23.241	68.605	12062.	-236564.	-190399.	19.162
550.	11.096	71.109	45.787	25.322	56.889	13927.	-236164.	-187655.	17.822
600.	11.120	75.942	48.102	27.840	54.818	16704.	-235839.	-183261.	15.954
631.	11.134	78.697	49.538	29.158	54.613	18399.	-235769.	-180547.	14.946
2 s	0.016	0.125	0.110	0.044	0.169	28.	156.	96.	0.008
				Ni(T_N)					
631.	11.134	78.697	49.538	29.158	54.613	18399.	-235769.	-180547.	14.945
650.	11.143	80.317	50.415	29.902	54.605	19436.	-235678.	-178886.	14.375
700.	11.167	84.367	52.697	31.670	54.727	22169.	-235359.	-174529.	13.023
750.	11.191	88.149	54.936	33.213	54.897	24910.	-235012.	-170196.	11.853
2 s	0.016	0.126	0.111	0.051	0.225	38.	162.	88.	0.006
800.	11.216	91.697	57.123	34.574	55.058	27659.	-234660.	-165886.	10.831
850.	11.240	95.039	59.256	35.782	55.208	30415.	-234313.	-161598.	9.930
900.	11.265	98.199	61.333	36.866	55.356	33179.	-233976.	-157331.	9.131
950.	11.290	101.196	63.353	37.843	55.511	35951.	-233651.	-153082.	8.417
1000.	11.314	104.048	65.317	38.731	55.683	38731.	-233339.	-148849.	7.775
2 s	0.016	0.148	0.112	0.096	0.407	96.	190.	70.	0.004
1050.	11.339	106.769	67.226	39.543	55.877	41520.	-233040.	-144632.	7.195
1100.	11.364	109.373	69.083	40.290	56.096	44319.	-232755.	-140429.	6.668
1150.	11.389	111.872	70.890	40.983	56.345	47130.	-232483.	-136239.	6.188
1200.	11.415	114.276	72.648	41.628	56.626	49954.	-232222.	-132060.	5.748
1250.	11.440	116.594	74.360	42.234	56.939	52793.	-231971.	-127892.	5.344
2 s	0.018	0.211	0.114	0.160	0.579	200.	263.	62.	0.003
1300.	11.465	118.834	76.027	42.807	57.286	55649.	-231730.	-123733.	4.972
1350.	11.490	121.003	77.653	43.350	57.666	58522.	-231497.	-119584.	4.627
1400.	11.516	123.107	79.239	43.869	58.080	61416.	-231270.	-115443.	4.307
1450.	11.541	125.153	80.787	44.366	58.527	64331.	-231049.	-111310.	4.010
1500.	11.566	127.145	82.299	44.846	59.006	67269.	-230831.	-107185.	3.732
2 s	0.021	0.301	0.124	0.231	0.912	346.	388.	94.	0.003
1550.	11.591	129.088	83.778	45.311	59.518	70232.	-230616.	-103067.	3.473
1600.	11.617	130.987	85.223	45.763	60.061	73221.	-230402.	-98956.	3.231
1650.	11.642	132.843	86.638	46.205	60.634	76239.	-230188.	-94852.	3.003
1700.	11.667	134.662	88.024	46.638	61.237	79285.	-229973.	-90754.	2.788
1728.	11.682	135.666	88.788	46.878	61.587	81005.	-229851.	-88462.	2.674
2 s	0.024	0.416	0.142	0.323	1.425	558.	586.	160.	0.005
				Ni(Crystal = Liquid)					
1728.	11.682	135.666	88.788	46.878	61.587	81005.	-247006.	-88462.	2.674
1750.	11.693	136.447	89.382	47.065	61.869	82363.	-246913.	-86444.	2.580
2 s	0.024	0.430	0.144	0.334	1.484	584.	611.	168.	0.005
1800.	11.718	138.199	90.714	47.484	62.528	85472.	-246680.	-81862.	2.376
2 s	0.025	0.463	0.150	0.361	1.624	650.	673.	188.	0.005

Table 8.18. Thermodynamic properties of oxygen, $O_2(g)$.

T	V°	S°	$-\frac{(G^\circ_T - H^\circ_{298})}{T}$	$\frac{(H^\circ_T - H^\circ_{298})}{T}$	C°_p	$H^\circ_T - H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
K	cm^3/mol	J/(mol·K)				J/mol			
200.	----	193.487	207.831	-14.345	28.818	-2869.	0.	0.	0.000
250.	----	199.990	205.635	-5.644	29.276	-1411.	0.	0.	0.000
273.15	----	202.584	205.268	-2.684	29.304	-733.	0.	0.	0.000
298.15	----	205.152	205.152	0.000	29.364	0.	0.	0.	0.000
300.	----	205.334	205.153	0.180	29.371	54.	0.	0.	0.000
350.	----	209.880	205.511	4.369	29.651	1529.	0.	0.	0.000
400.	----	213.867	206.312	7.555	30.083	3022.	0.	0.	0.000
450.	----	217.439	207.353	10.087	30.588	4539.	0.	0.	0.000
500.	----	220.689	208.526	12.162	31.113	6081.	0.	0.	0.000
550.	----	223.678	209.770	13.909	31.626	7650.	0.	0.	0.000
600.	----	226.451	211.046	15.405	32.114	9243.	0.	0.	0.000
650.	----	229.040	212.331	16.709	32.568	10861.	0.	0.	0.000
700.	----	231.469	213.612	17.857	32.987	12500.	0.	0.	0.000
750.	----	233.758	214.880	18.879	33.373	14159.	0.	0.	0.000
800.	----	235.923	216.128	19.795	33.725	15836.	0.	0.	0.000
850.	----	237.978	217.353	20.625	34.049	17531.	0.	0.	0.000
900.	----	239.932	218.554	21.379	34.345	19241.	0.	0.	0.000
950.	----	241.797	219.729	22.068	34.617	20965.	0.	0.	0.000
1000.	----	243.579	220.877	22.702	34.867	22702.	0.	0.	0.000
1050.	----	245.286	221.999	23.287	35.098	24451.	0.	0.	0.000
1100.	----	246.923	223.095	23.828	35.311	26211.	0.	0.	0.000
1150.	----	248.497	224.165	24.332	35.509	27982.	0.	0.	0.000
1200.	----	250.013	225.211	24.802	35.693	29762.	0.	0.	0.000
1250.	----	251.473	226.232	25.241	35.865	31551.	0.	0.	0.000
1300.	----	252.883	227.230	25.652	36.025	33348.	0.	0.	0.000
1350.	----	254.246	228.206	26.040	36.176	35154.	0.	0.	0.000
1400.	----	255.564	229.160	26.404	36.318	36966.	0.	0.	0.000
1450.	----	256.841	230.092	26.748	36.452	38785.	0.	0.	0.000
1500.	----	258.079	231.005	27.074	36.579	40611.	0.	0.	0.000
1550.	----	259.280	231.897	27.383	36.700	42443.	0.	0.	0.000
1600.	----	260.447	232.771	27.676	36.815	44281.	0.	0.	0.000
1650.	----	261.581	233.627	27.954	36.925	46124.	0.	0.	0.000
1700.	----	262.685	234.466	28.219	37.030	47973.	0.	0.	0.000
1750.	----	263.760	235.287	28.473	37.131	49827.	0.	0.	0.000
1800.	----	264.808	236.093	28.714	37.228	51686.	0.	0.	0.000

Table 8.19. Thermodynamic properties of silicon, Si(s,l).

T	V°	S°	$\frac{-(G^\circ_T-H^\circ_{298})}{T}$	$\frac{(H^\circ_T-H^\circ_{298})}{T}$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
K	cm^3/mol	---J/(mol·K)---				---J/mol---			
200.	----	11.648	20.521	-8.875	15.588	-1775.	0.	0.	0.000
250.	----	15.440	19.130	-3.692	18.271	-923.	0.	0.	0.000
273.15	----	17.097	18.888	-1.790	19.154	-489.	0.	0.	0.000
298.15	----	18.810	18.810	0.000	19.946	0.	0.	0.	0.000
300.	----	18.934	18.810	0.123	19.999	37.	0.	0.	0.000
350.	----	22.113	19.059	3.054	21.222	1069.	0.	0.	0.000
400.	----	25.010	19.624	5.385	22.146	2154.	0.	0.	0.000
450.	----	27.662	20.372	7.289	22.875	3280.	0.	0.	0.000
500.	----	30.104	21.225	8.878	23.470	4439.	0.	0.	0.000
550.	----	32.365	22.136	10.229	23.970	5626.	0.	0.	0.000
600.	----	34.469	23.077	11.392	24.398	6835.	0.	0.	0.000
650.	----	36.437	24.030	12.408	24.771	8065.	0.	0.	0.000
700.	----	38.285	24.983	13.303	25.100	9312.	0.	0.	0.000
750.	----	40.027	25.928	14.099	25.394	10574.	0.	0.	0.000
800.	----	41.675	26.861	14.814	25.659	11851.	0.	0.	0.000
850.	----	43.238	27.779	15.459	25.901	13140.	0.	0.	0.000
900.	----	44.724	28.680	16.044	26.122	14440.	0.	0.	0.000
950.	----	46.142	29.562	16.581	26.327	15752.	0.	0.	0.000
1000.	----	47.498	30.425	17.073	26.517	17073.	0.	0.	0.000
1050.	----	48.796	31.269	17.527	26.693	18403.	0.	0.	0.000
1100.	----	50.041	32.094	17.947	26.859	19742.	0.	0.	0.000
1150.	----	51.239	32.901	18.338	27.015	21089.	0.	0.	0.000
1200.	----	52.392	33.689	18.703	27.162	22443.	0.	0.	0.000
1250.	----	53.503	34.459	19.044	27.302	23805.	0.	0.	0.000
1300.	----	54.577	35.213	19.364	27.435	25173.	0.	0.	0.000
1350.	----	55.614	35.949	19.665	27.561	26548.	0.	0.	0.000
1400.	----	56.619	36.669	19.949	27.682	27929.	0.	0.	0.000
1450.	----	57.592	37.374	20.218	27.797	29316.	0.	0.	0.000
1500.	----	58.537	38.064	20.473	27.908	30709.	0.	0.	0.000
1550.	----	59.454	38.739	20.714	28.015	32107.	0.	0.	0.000
1600.	----	60.345	39.401	20.944	28.118	33510.	0.	0.	0.000
1650.	----	61.211	40.048	21.163	28.217	34919.	0.	0.	0.000
1685.	----	61.804	40.494	21.310	28.285	35908.	0.	0.	0.000
				Si(Crystal = Liquid)					
1685.	----	91.805	40.494	51.311	25.522	86459.	0.	0.	0.000
1700.	----	92.031	40.948	51.083	25.522	86841.	0.	0.	0.000
1750.	----	92.771	42.418	50.353	25.522	88117.	0.	0.	0.000
1800.	----	93.490	43.827	49.663	25.522	89394.	0.	0.	0.000

Table 8.20. Thermodynamic properties of cristobalite ("s1=low=alpha","s2=high=beta"), SiO_2(s1,s2).

T K	V° cm^3/mol	S°	$-(G^\circ_T-H^\circ_{298})/T$	$(H^\circ_T-H^\circ_{298})/T$	C°_p	$H^\circ_T-H^\circ_{298}$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log {}_f K^\circ$
		------------J/(mol·K)------------				--------J/mol--------			
200.	25.509	27.867	47.145	-19.280	32.919	-3856.	-907275.	-871822.	227.692
250.	25.637	35.950	44.103	-8.152	39.586	-2038.	-907767.	-862898.	180.289
273.15	25.693	39.575	43.566	-3.990	42.269	-1090.	-907931.	-858735.	164.213
298.15	25.751	43.392	43.392	0.000	44.897	0.	-908063.	-854226.	149.654
300.	25.755	43.671	43.393	0.277	45.081	83.	-908071.	-853892.	148.673
350.	25.865	50.968	43.959	7.009	49.562	2453.	-908208.	-844849.	126.084
400.	25.967	57.834	45.269	12.565	53.237	5026.	-908213.	-835796.	109.141
450.	26.063	64.285	47.027	17.258	56.278	7766.	-908116.	-826749.	95.965
500.	26.153	70.350	49.059	21.290	58.816	10645.	-907938.	-817717.	85.425
543.	26.227	75.280	50.942	24.337	60.672	13215.	-907735.	-809966.	77.914
				(alpha) = (beta)					
543.	27.264	77.724	50.942	26.783	59.421	14543.	-906407.	-809966.	77.914
550.	27.270	78.487	51.288	27.200	59.785	14960.	-906379.	-808723.	76.805
600.	27.309	83.790	53.777	30.013	62.037	18008.	-906134.	-799856.	69.632
650.	27.342	88.828	56.281	32.546	63.804	21155.	-905833.	-791011.	63.565
700.	27.370	93.610	58.778	34.831	65.220	24382.	-905492.	-782191.	58.367
750.	27.393	98.151	61.253	36.897	66.374	27673.	-905123.	-773397.	53.863
800.	27.413	102.466	63.695	38.770	67.331	31016.	-904733.	-764628.	49.924
850.	27.430	106.572	66.098	40.475	68.134	34404.	-904330.	-755883.	46.450
900.	27.444	110.487	68.456	42.031	68.818	37828.	-903916.	-747163.	43.363
950.	27.456	114.224	70.767	43.457	69.407	41284.	-903496.	-738466.	40.603
1000.	27.466	117.797	73.030	44.767	69.919	44767.	-903070.	-729791.	38.120
1050.	27.475	121.220	75.244	45.976	70.369	48275.	-902643.	-721138.	35.874
1100.	27.482	124.503	77.409	47.094	70.768	51803.	-902213.	-712505.	33.833
1150.	27.489	127.656	79.525	48.131	71.123	55351.	-901783.	-703891.	31.971
1200.	27.494	130.690	81.594	49.096	71.444	58915.	-901353.	-695297.	30.265
1207.45	27.494	131.133	81.899	49.234	71.489	59448.	-901289.	-694017.	30.023
				-Quartz(beta) = Cristobalite(beta)					
1207.45	27.494	131.133	81.899	49.234	71.489	59448.	-901289.	-694017.	30.023
1250.	27.498	133.613	83.617	49.996	71.734	62495.	-900924.	-686720.	28.696
1300.	27.502	136.431	85.594	50.837	71.998	66088.	-900497.	-678160.	27.248
1350.	27.505	139.153	87.528	51.625	72.241	69694.	-900071.	-669617.	25.908
1400.	27.508	141.785	89.419	52.366	72.465	73312.	-899647.	-661089.	24.665
1450.	27.510	144.331	91.269	53.062	72.673	76940.	-899224.	-652577.	23.508
1500.	27.512	146.798	93.079	53.719	72.867	80579.	-898804.	-644079.	22.428
1550.	27.514	149.190	94.851	54.340	73.048	84227.	-898386.	-635595.	21.419
1600.	27.515	151.512	96.585	54.928	73.219	87884.	-897971.	-627124.	20.473
1650.	27.516	153.768	98.284	55.484	73.380	91549.	-897558.	-618667.	19.585
1685.	27.517	155.309	99.452	55.857	73.488	94119.	-897270.	-612754.	18.995
				Si(Crystal = Liquid)					
1685.	27.517	155.309	99.452	55.857	73.488	94119.	-947821.	-612754.	18.995
1700.	27.517	155.961	99.948	56.012	73.533	95221.	-947656.	-609772.	18.736
1750.	27.518	158.094	101.579	56.515	73.678	98902.	-947106.	-599842.	17.904
1800.	27.519	160.172	103.178	56.994	73.816	102589.	-946554.	-589928.	17.119

Table 8.21. Thermodynamic properties of quartz ("s1=low=alpha","s2=high=beta"), SiO_2(s1,s2).

T K	$V°$ cm^3/mol	$S°$	$-(G°_T-H°_{298})/T$	$(H°_T-H°_{298})/T$	$C°_p$	$H°_T-H°_{298}$	$\Delta_f H°$	$\Delta_f G°$	$\log {}_f K°$
		J/(mol·K)				J/mol			
200.	22.631	26.046	45.177	-19.130	32.649	-3826.	-909885.	-874067.	228.278
250.	22.663	34.067	42.158	-8.092	39.279	-2023.	-910391.	-865050.	180.739
273.15	22.680	37.664	41.625	-3.961	41.946	-1082.	-910562.	-860844.	164.616
298.15	22.701	41.453	41.453	0.000	44.586	0.	-910702.	-856287.	150.015
300.	22.702	41.729	41.453	0.277	44.773	83.	-910710.	-855949.	149.031
350.	22.747	48.988	42.016	6.971	49.403	2440.	-910860.	-846808.	126.377
400.	22.797	55.851	43.321	12.530	53.378	5012.	-910866.	-837656.	109.384
450.	22.852	62.342	45.077	17.264	56.837	7769.	-910752.	-828510.	96.169
500.	22.909	68.491	47.113	21.378	59.880	10689.	-910534.	-819383.	85.599
550.	22.970	74.327	49.324	25.004	62.580	13752.	-910226.	-810282.	76.953
600.	23.034	79.878	51.641	28.237	64.990	16942.	-909838.	-801213.	69.750
650.	23.100	85.167	54.018	31.149	67.154	20247.	-909381.	-792179.	63.659
700.	23.167	90.216	56.425	33.791	69.104	23654.	-908859.	-783183.	58.441
750.	23.236	95.045	58.840	36.205	70.868	27154.	-908281.	-774225.	53.921
800.	23.307	99.670	61.248	38.423	72.467	30738.	-907651.	-765309.	49.968
845.50	23.372	103.716	63.425	40.291	73.796	34066.	-907037.	-757230.	46.780
				(alpha) = (beta)					
845.50	23.668	104.767	63.425	41.341	68.716	34954.	-906148.	-757230.	46.780
850.	23.669	105.131	63.645	41.486	68.702	35263.	-906109.	-756438.	46.484
900.	23.683	109.056	66.060	42.996	68.635	38696.	-905687.	-747646.	43.391
950.	23.695	112.768	68.421	44.346	68.701	42129.	-905289.	-738877.	40.625
1000.	23.705	116.296	70.728	45.568	68.869	45568.	-904909.	-730128.	38.137
1050.	23.714	119.661	72.978	46.683	69.118	49017.	-904539.	-721398.	35.887
1100.	23.721	122.884	75.174	47.710	69.430	52481.	-904174.	-712686.	33.842
1150.	23.727	125.978	77.316	48.662	69.793	55961.	-903812.	-703990.	31.976
1200.	23.732	128.957	79.406	49.551	70.195	59461.	-903447.	-695309.	30.265
1207.45	23.733	129.391	79.713	49.678	70.258	59984.	-903392.	-694017.	30.023
				-Quartz(beta) = Cristobalite(beta)					
1207.45	23.733	129.391	79.713	49.678	70.258	59984.	-903392.	-694017.	30.023
1250.	23.737	131.831	81.446	50.385	70.631	62981.	-903077.	-686645.	28.693
1300.	23.740	134.610	83.438	51.172	71.092	66524.	-902699.	-677995.	27.242
1350.	23.744	137.302	85.383	51.919	71.573	70091.	-902313.	-669360.	25.899
1400.	23.746	139.914	87.284	52.630	72.072	73682.	-901915.	-660739.	24.652
1450.	23.749	142.452	89.143	53.309	72.584	77298.	-901505.	-652133.	23.492
1500.	23.751	144.921	90.961	53.960	73.107	80940.	-901082.	-643541.	22.410
1550.	23.752	147.327	92.741	54.586	73.639	84609.	-900643.	-634963.	21.398
1600.	23.753	149.674	94.483	55.190	74.177	88304.	-900189.	-626400.	20.449
1650.	23.755	151.964	96.191	55.774	74.721	92027.	-899718.	-617852.	19.559
1685.	23.755	153.537	97.366	56.172	75.105	94649.	-899379.	-611876.	18.968
				Si(Crystal = Liquid)					
1685.	23.755	153.537	97.366	56.172	75.105	94649.	-949930.	-611876.	18.968
1700.	23.756	154.203	97.864	56.339	75.270	95777.	-949740.	-608868.	18.708
1750.	23.756	156.393	99.505	56.888	75.821	99554.	-949093.	-598851.	17.874
1800.	23.757	158.537	101.115	57.422	76.376	103359.	-948423.	-588854.	17.088

Table 8-22.

IRON Molar mass 55.847 g•mol^{-1}

Fe: Alpha crystals (body-centered cubic) 298.15 to 1184 K. Curie point 1043.2 K. Gamma crystals (face-centered cubic) 1184 to 1665 K. Alpha crystals 1665 K to melting point 1809 K.

Temp. T	Heat capacity C_P°	Entropy S_T°	Enthalpy function $(H_T^\circ-H_{298}^\circ)/T$	Gibbs energy function $-(G_T^\circ-H_{298}^\circ)/T$	Formation from elements Enthalpy	Formation from elements Gibbs energy
K	J•mol^{-1}•K^{-1}	J•mol^{-1}•K^{-1}	J•mol^{-1}•K^{-1}	J•mol^{-1}•K^{-1}	kJ•mol^{-1}	kJ•mol^{-1}
298.15	25.15	27.319	0.000	27.319	0.	0.
	±0.07	±0.002				
300	25.20	27.475	0.155	27.319	0.	0.
350	26.36	31.449	3.817	27.632	0.	0.
400	27.40	35.037	6.700	28.337	0.	0.
450	28.42	38.322	9.058	29.264	0.	0.
500	29.48	41.371	11.046	30.325	0.	0.
550	30.62	44.233	12.773	31.460	0.	0.
600	31.87	46.950	14.310	32.640	0.	0.
650	33.25	49.554	15.714	33.840	0.	0.
700	34.80	52.074	17.020	35.054	0.	0.
750	36.56	54.533	18.263	36.270	0.	0.
800	38.59	56.955	19.468	37.487	0.	0.
850	41.00	59.365	20.661	38.704	0.	0.
900	44.00	61.790	21.871	39.919	0.	0.
950	48.08	64.271	23.137	41.134	0.	0.
1000	54.88	66.891	24.535	42.356	0.	0.
1043.2	70.73	69.474	26.050	43.424	0.	0.
1043.2	70.73	69.474	26.050	43.424	0.	0.
1100	45.31	72.126	27.286	44.840	0.	0.
1184	41.27	75.285	28.393	46.892	0.	0.
1184	34.31	76.085	29.193	46.892	0.	0.
1200	34.41	76.546	29.262	47.284	0.	0.
1300	35.09	79.327	29.684	49.643	0.	0.
1400	35.77	81.953	30.094	51.859	0.	0.
1500	36.47	84.444	30.496	53.948	0.	0.
1600	37.16	86.820	30.891	55.929	0.	0.
1665	37.61	88.309	31.145	57.164	0.	0.
1665	40.13	88.811	31.647	57.164	0.	0.
1700	40.34	89.648	31.824	57.824	0.	0.
1800	41.02	91.973	32.316	59.657	0.	0.
1809	41.09	92.178	32.359	59.819	0.	0.
1809	43.19	99.832	40.014	59.819	0.	0.
1900	43.48	101.959	40.173	61.786	0.	0.
2000	43.78	104.197	40.346	63.851	0.	0.
	±1.00	±0.078				

$H_{298}^\circ - H_0^\circ$ 4.489 ±0.015 kJ•mol^{-1} Molar volume 0.7092 ±0.0001 J•bar^{-1}•mol^{-1}

Transitions in phase

Transition in reference state elements

Curie point	1043.2	K
α - γ	1184	K
Enthalpy	0.948	kJ•mol^{-1}
γ - α	1665	K
Enthalpy	0.836	kJ•mol^{-1}
Melting point	1809	K
Enthalpy	13.848	

Recommended Standard Electrochemical Potentials and Fugacities of Oxygen for the Solid Buffers and Thermodynamic Data in the System Iron-Silicon-Oxygen, Nickel-Oxygen, and Copper-Oxygen

Part 6. FORTRAN Source Code for TDM001

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May 28, 1990

The source computer code listed in this section is the PC version of the program used to generate the data given in Parts 1-5. The code is given in two sections, PARAM.FOR and TDM001.FOR. PARAM.FOR is inserted at compile time by an INCLUDE statement in TDM001.FOR. The version compiles in 600K bytes. The version works except for the section dealing with the Grueneisen constant. The Grueneisen constant is calculated in subroutine MISCFN, but cannot be used in any refinement because the derivatives of gamma with respect to each of the fitted constants has not been programmed.

```
C
-----------------------------------------------------------------------
C
C      PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C       IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C        DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C        MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C        ALSO.
C
C
-----------------------------------------------------------------------
      PARAMETER (IP1=   4)      ! MAX. NO. OF PHASES IN PROBLEM.
      PARAMETER (IP2=3000)      ! MAX. NO. OF OBSERVATIONS.
      PARAMETER (IP3= 250)      ! MAX. NO. OF DATA SETS.
      PARAMETER  (IP4=     4)        !  MAX.  NO.  OF  PHASES  PER
OBSERVATION.
      PARAMETER (IP5=IP4+1)     ! SPECIAL.  USED IN "PUTPUT".
      PARAMETER  (NX=6)              !  MAX.  NO.  OF  INDEPENDENT
VARIABLES.
      PARAMETER  (NCPARM=10)       !  NO.  OF  CONSTANTS  IN  THERMAL
FUNCTIONS.
      PARAMETER  (NMPARM=4)       !  NO.  OF  CONSTANTS  FOR  MAGNETIC
ANOMALY.
      PARAMETER  (NVPARM=8)         !  NO.  OF  CONSTANTS  IN  VOLUME
FUNCTION.
      PARAMETER (NLPARM=3)      ! NO. OF INTEGER CONST. IN LAMBDA
ANOM.
      PARAMETER (NPARM=NCPARM+NMPARM+NVPARM+NLPARM) !TOTAL NO. OF
CONST.
      PARAMETER (IP6=NPARM*IP1) ! MAXINUM NO. OF CONSTANTS.
      PARAMETER (IP7=IP6/1)      ! MAXINUM NO. OF CONSTANTS TO BE
FIT.
C  SPACE MAY BE SAVED BY ADJUSTING THE DIVISOR IN THE DEFINITION OF
C      "IP7"  TO  FIT  ONLY  A  FRACTION  OF  THE  MAXIMUM  NUMBER  OF
CONSTANTS
C    IN THE PROBLEM.  WITH THE DIVISOR SET TO 1, ALL CONSTANTS MAY
C    BE FIT IN THE PROBLEM.
      PARAMETER (IP8=IP7*(IP7+3)/2) ! SPECIAL.  USED IN "MINV".
      PARAMETER (IP9=28)        ! NO. OF LABELS FOR DATA TYPES.
      PARAMETER  (IP10=2)           !  MAX.  NO.  OF  TRANSITIONS  IN
SERIES.
      PARAMETER (IP11=IP10+1)   ! MAX. NO. OF PHASES IN TRANSITION
SERIES.
C
-----------------------------------------------------------------------
C     END OF PARAMETER STATEMENTS.
```

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C
----------------------------------------------------------------------
C
                                      PROGRAM TDM001
C
C                        VERSION MARCH, 1990 BY J.L. HAAS, JR.
C
C                                      INTRODUCTION
C
C    TDM  IS  A  FORTRAN  PROGRAM  FOR  SIMULTANEOUS  FITTING  OF
THERMODYNAMIC
C     DATA (TYPES GIVEN UNDER CAPABILITY, BELOW) FOR A GIVEN SET OF
C      PHASES WITHIN A CHEMICAL SYSTEM.  TDM IS THE ACRONYM FOR
C      "THERMODYNAMIC DATA OF MINERALS" AND IS PRONOUNCED "TE' DE
UM" OR
C      "TEDIUM".  TDM IS A COMPLETE REVISION OF THE OLDER "PHAS20"
C      PROGRAM.  THE REVISION ALLOWS FOR 6 INDEPENDENT VARIABLES
C      INCLUDING THE TEMPERATURE OF THE OBSERVATION, A REFERENCE
C      TEMPERATURE FOR THE SAME OBSERVATION IF APPLICABLE,
C     THE PRESSURE OF THE OBSERVATION, A REFERENCE PRESSURE FOR THE
C     SAME OBSERVATION IF APPLICABLE, AND TWO UNASSIGNED VARIABLES.
THE
C       ROUTINE ACCOMPLISHES THE FITTING OF PROPERTIES RELATED TO
VOLUME
C       AND ENERGY FOR A GROUP OF CHEMICALLY RELATED PHASES, AND
VOLUME
C      AND ENERGY EFFECTS ASSOCIATED WITH LAMBDA ANOMALIES DUE TO
C       MAGNETIC DISORDERING.  THE SAME FUNCTIONS SHOULD FIT THE
VOLUME
C          AND  ENERGY  EFFECTS  ASSICIATED  WITH  CRYSTALLOGRAPHIC
DISORDERING
C      BUT THIS HAS NOT BEEN TESTED.
C
C  THIS VERSION WILL HANDLE:
C                    4 PHASES, THE PROPERTIES BEING EITHER FIXED OR
REFINED.
C              3000 INDEPENDENT OBSERVATIONS CONTAINED IN
C               250 DATA SETS. EACH SET CAN CONTAIN MEASURED
C                   OBSERVATIONS THAT MAY BE CALCULATED FROM
C                   THE PROPERTIES OF FROM 1 TO A MAXIMUM OF
C                 4 PHASES.
C      THE PROGRAM MAY BE ADAPTED TO THE CAPABILITY OF PARTICULAR
C         COMPUTERS  OR  TO  LARGER  PROBLEMS  IN  THERMODYNAMICS  BY
DECREASING
C         OR  INCREASING  THE  DIMENSIONS  PROVIDED  IN  "PARAMETER"
STATEMENTS.
C     THESE ARE FOUND IN THE COMPANION FILE "PARAM.FOR".  "INCLUDE"
C      STATEMENTS IN EACH ROUTINE READS IN "PARAM.FOR" DURING
C      COMPILATION.
C
C
C                                 HISTORICAL BACKGROUND
C
C  CHEMICAL AND PHYSICAL MODELLING OF NATURAL PROCESSES REQUIRES
```

```
C      ACCURATE THERMODYNAMIC DATA.  TDM (AND THE OLDER VERSION
PHAS20)
C     WAS WRITTEN TO FILL A NEED FOR COMPUTER-ORIENTED EVALUATION
OF
C     THERMODYNAMIC DATA OF ALL TYPES TO INSURE THAT THE RESULTS
ARE
C     CONSISTENT WITH THE PROPERTY OF INTEREST AND ALSO WITH ALL
THE
C     PROPERTIES DERIVED FROM THE PROPERTY OF INTEREST THROUGH
C     APPLICATION OF THE LAWS OF THERMODYNAMICS.
C
C
C                              CAPABILITY
C
C   TDM CAN BE USED TO FIT ONE OR MORE OF THE FOLLOWING
THERMOPHYSICAL
C     AND THERMOCHEMICAL PROPERTIES.  THE TERMS T AND P REPRESENT
THE
C     TEMPERATURE AND PRESSURE OF THE OBSERVATION.  THE TERMS TR
AND PR
C     REPRESENT A REFERENCE TEMPERATURE AND PRESSURE FOR THE
C     OBSERVATION.
C
C    CP(T,1) AND DELTA CP(T,1)          HEAT CAPACITY AT CONSTANT
C                                           PRESSURE,
C     CP(T,1)-CP(TR,1)                    ---
C     CV(T,1)                            HEAT CAPACITY AT CONSTANT
C                                           VOLUME,
C     S(T,1) AND DELTA S(T,1)             ENTROPY,
C     S(T,1)-S(TR,1)                      ---
C     H(T,1) AND DELTA H(T,1)             ENTHALPY,
C    DELTA H(SOLUTION)                  ENTHALPY OF SOLUTION WHERE
A
C                                              SOLUTION AT T AND A
SOLID AT
C                                          TR ARE REACTED.  TR MAY
BE
C                                            THE SAME AS OR DIFFER
FROM T.
C     H(T,1)-H(TR,1)                      INCREMENTAL ENTHALPY OR
HEAT
C                                           CONTENT,
C     G(T,1) AND DELTA G(T,1)             GIBBS ENERGY,
C     G(T,1)-G(TR,1)                      ---
C     [G(T,1)-H(TR,1)]/T                  GIBBS ENERGY FUNCTION
C     LOG K                               EQUILIBRIUM CONSTANT,
C     E                                  ELECTROCHEMICAL POTENTIAL,
C     V(T,P) AND DELTA V(T,P)             VOLUME,
C      V(T,P)-V(TR,PR)                        VOLUME RELATIVE TO A
REFERENCE
C                                           VOLUME,
C    V(T,P)/V(TR,PR)                     REDUCED VOLUME AT CONSTANT
C                                           PRESSURE,
C     ALPHA(T,P)                          COEFFICIENT OF VOLUME
```

```
C                                                 EXPANSION,
C       [V(T,P)-V(TR,P)]/V(TR,P)                     RELATIVE VOLUME AT
CONSTANT
C                                                 PRESSURE,
C      [V(T,P)-V(TR,P)]/[V(TR,P)*(T-TR)]  APPARENT COEFFICIENT OF
VOLUME
C                                                 EXPANSION,
C     KAPPA-S(T,P)                              COEFFICIENT OF VOLUME
C                                               COMPRESSION AT CONSTANT
C                                                 ENTROPY,
C     KAPPA-T(T,P)                              COEFFICIENT OF VOLUME
C                                               COMPRESSION AT CONSTANT
C                                                 TEMPERATURE,
C     BMS(T,P)                                  ISENTROPIC BULK MODULUS
C                                                 [=1/KAPPA-S]
C     BMT(T,P)                                  ISOTHERMAL BULK MODULUS
C                                                 [=1/KAPPA-T]
C       [V(T,P)-V(T,PR)]/V(T,PR)                     RELATIVE VOLUME AT
CONSTANT
C                                                 TEMPERATURE,
C      [V(T,P)-V(T,PR)]/[V(T,PR)*(P-PR)]  APPARENT COEFFICIENT OF
VOLUME
C                                                 COMPRESSION,
C     G(T,P) AND DELTA G(T,P)                   GIBBS ENERGY AT ELEVATED
C                                                PRESSURE  (REQUIRES THE
C                                                 CALCULATION OF VOLUME
C                                               DIFFERENCES AT T AND P),
C      dP/dT AT P = 0.0                             PRESSURE COEFFICIENT
(SLOPE OF
C                                                     P-T CURVES AT 0
PRESSURE,
C     T(CRIT)                                   CRITICAL TEMPERATURES AS
A
C                                                 FUNCTION OF PRESSURE.
C     GAMMA                                   GRUENEISEN CONSTANT (to be
programmed).
C
C
C                                BASIC FUNCTIONS
C
C  TO BE SUCCESSFUL, THE MATHEMATICAL MODEL MUST BE CAPABLE OF
FITTING
C     THE MOST SENSITIVE MEASUREMENT MADE ON A CHEMICAL OR PHYSICAL
C     SYSTEM.  IN THIS SITUATION, THIS MEANS THAT THE MODEL MUST BE
C      CAPABLE OF FITTING (1) THE HEAT CAPACITY OF THE PHASES OF
C      INTEREST AT THE REFERENCE PRESSURE AND (2) THE COEFFICIENTS
OF
C     VOLUME COMPRESSION AND VOLUME EXPANSION AT ALL P AND T.  THE
C      FUNCTIONS MUST BE CAPABLE OF INTEGRATION TO DERIVE ENTROPY,
C      ENTHALPY, GIBBS ENERGY AND VOLUME.
C
C
C                          FUNCTION FOR HEAT CAPACITY
C
```

```
C  THE FOLLOWING POLYNOMIAL HAS BEEN PROGRAMMED TO FIT THE HEAT
C      CAPACITIES OF MOST SUBSTANCES:
C
C  Cp = A1*T**-3 + A2*T**-2 + A3*T**-1 + A4*T**-.5 + A5 + A6*T +
C      A7*T**2 + A8*T**3 + CP(ANOMALY)
C
C  THE USE OF CONSTANTS A1 THROUGH A8 IS SELECTED BY THE OPERATOR.
NO PHASE
C      REQUIRES ALL CONSTANTS.  ATTEMPTS TO FIT ALL CONSTANTS WILL
LEAD
C          TO  SINGULARITIES  BECAUSE  GROSS  OVERFITTING  IS  BEING
ATTEMPTED.
C     THE LAST TERM "CP(ANOMALY)" IS ADDED TO COVER SUCH PHENOMENON
AS
C         MAGNETIC  DISORDERING  OR  STRUCTURAL  DISORDERING.   THE
MEIER-KELLEY
C      EQUATION USES A5, A6, AND A3.  THE HAAS-FISHER EQUATION USES
A2,
C       A4,  A5,  A6,  AND  A7  BUT  THESE  ARE  MORE  THAN  ARE  NECESSARY.
THE
C      BERMAN-BROWN EQUATION USES A1, A2, A4, AND A5 BUT A2 AND A4
MUST
C      BE CONSTRAINED TO BE NEGATIVE.  THE FEI-SAXENA EQUATION USES
C      "3RN" PLUS THE CONSTANTS A1, A2, A3, A5, AND A6.  THE TERM
"3RN"
C     REPRESENTS THE PETIT-DULONG LIMIT FOR SOLIDS WHERE "R" IS THE
GAS
C      CONSTANT  AND  "N"  IS  THE  NUMBER  OF  ATOMS  IN  THE  SOLID.   THE
CODATA
C      EQUATION USES A2, A3, A5, A6, A7, AND A8 BUT THE INDEPENDENT
C      VARIABLE IS "X=10**-4*T" IN PLACE OF T AS USED HERE.
C
C   FOR  MAGNETIC  DISORDERING,  THE  FOLLOWING  FUNCTIONS  HAVE  BEEN
USEFUL.
C      FOR T LESS THAN OR EQUAL TO T(CRIT),
C
C                    JN
C  CP(M) = A13*SUMM TAU**[JA*(2K-1)]/(2K-1).
C                   K=1
C
C      FOR T GREATER THAN T(CRIT),
C
C                    JN
C  CP(M) = A14*SUMM TAU**[JB*(2K-1)]/(2K-1).
C                   K=1
C
C      "TAU"  IS  EQUAL  TO  T/T(CRIT).   IN  THE  ABOVE  EXPRESSIONS  FOR
CP(M),
C     THE FIRST TRIAL CONSTANTS FOR "JA" AND "JB" SHOULD BE +3 AND
-5,
C       RESPECTIVELY.   THE  NUMBER  OF  TERMS,  "JN",  SHOULD  BE  7  OR
GREATER.
C        FOR  FURTHER  INFORMATION  REFER  TO  INDEN  (1981),  PHYSICA,
103B:82-100.
```

```
C
C
C             FUNCTION FOR THE COEFFICIENT OF VOLUME EXPANSION
C
C  THE COEFFICIENT OF VOLUME EXPANSION OF SOLIDS IS FIT BY THE
C     FOLLOWING EQUATION:
C
C  ALPHA = B1 + B2*T + B3*EXP(-T/B8)
C
C       BECAUSE THE COEFFICIENT OF VOLUME EXPANSION FOR SOLIDS
APPROACHES
C     A CONSTANT AT EXTREME TEMPERATURES, B2 SHOULD BE USED ONLY
C        SPARINGLY.  THE CONSTANT B8 MUST BE SUPPLIED BY THE
EVALUATOR.  A
C     FIRST ESTIMATE WOULD BE A CONSTANT OF THE MAGNITUDE 1.5*T(D)
WHERE
C     T(D) IS THE DEBYE TEMPERATURE.  TRIAL ADJUSTMENTS REVISING
C     THAT ESTIMATE ARE THE OPTIONS OF THE USER.  THE PROGRAM IS
NOT SET
C     TO OPTIMIZE THE CONSTANT B8.
C
C
C                  FUNCTIONS FOR THE BULK MODULUS AND THE
C                     COEFFICIENT OF VOLUME COMPRESSION
C
C   THE COEFFICIENT OF VOLUME COMPRESSION AT CONSTANT TEMPERATURE
IS
C     EQUAL TO THE RECIPROCAL OF THE ISOTHERMAL BULK MODULUS.  THE
C       ISOTHERMAL BULK MODULUS AT ZERO PRESSURE IS FIT BY THE
FOLLOWING
C     EXPRESSION:
C
C  BMT(T,P=0) = B4 + B5*T
C
C     THE GENERAL EQUATION FOR THE BULK MODULUS IS AS FOLLOWS:
C
C  BMT(T,P) = BMT(T,P=0) + B6*P
C
C
C                            FUNCTION FOR VOLUME
C
C  THE GENERAL EQUATION FOR THE VOLUME OF A SOLID PHASE IS GIVEN BY
THE
C     FOLLOWING EQUATION:
C
C   V(T,P)  =  {B7*EXP[B1*T  +  B2*T**2/2  -  B3*B8*EXP(-T/B8)]  +
V(ANOMALY)}
C
C     *[1 + B6*P/K(T,P=0)]**-(1/B6)
C
C  THE LAST PRODUCT IS THE MURNAGHAN EQUATION OF STATE WITH THE
C        MODIFICATION THAT THE ISOTHERMAL BULK MODULUS AT ZERO
PRESSURE IS
C     A LINEAR FUNCTION OF TEMPERATURE.
```

```
C
C  FOR MAGNETIC DISORDERING, THE VOLUMETRIC ANOMALY WAS MODELLED AS
A
C        CONTRIBUTION PROPORTIONAL TO THE ENTHALPY OF MAGNETIC
DISORDERING,
C     H(M).  THIS AGREED WELL WITH THE OBSERVED VOLUMETRIC DATA FOR
IRON
C       AND FOR THE SLOPE OF THE CRITICAL TEMPERATURE OF IRON,
T(CRIT),
C      WITH PRESSURE.
C
C  V(M) = A12 * H(M)
C
C  T(CRIT) = A11*[1 + 0.1*A12*(P - 1)]
C
C     THE CONSTANT A11 IS THE CRITICAL TEMPERATURE AT THE REFERENCE
C      PRESSURE.  THE USER MUST ASSIGN THIS VALUE.  THE PROGRAM IS
NOT
C      SET TO OPTIMIZE THE CONSTANT A11.  THE CONSTANT A12 IS THE
SLOPE
C       OF THE CRITICAL CURVE WITH PRESSURE.  THE PROGRAM WILL
OPTIMIZE
C      ON THIS VALUE PROVIDED (1) DATA FOR THE CRITICAL TEMPERATURE
AS A
C      FUNCTION OF PRESSURE ARE SUPPLIED, (2) DATA FOR THE MOLAR
VOLUMES
C      AS A FUNCTION OF TEMPERATURE ARE SUPPLIED BOTH ABOVE AND
BELOW
C      THE CRITICAL TEMPERATURE AT THE REFERENCE PRESSURE, OR (3) A
C      COMBINATION OF THE ABOVE SETS OF DATA ARE AVAILABLE.
C
C
C                               REFERENCE STATES
C
C  THE REFERENCE STATE FOR ENTROPY IS THE PERFECT CRYSTAL AT 0 K.
FOR
C      THIS STATE, S = 0.0 J/(MOL K).
C
C  THE REFERENCE STATE FOR ENTHALPY IS THE STABLE STRUCTURE AT
298.15 K
C     AND 1 BAR (10**5 GPA).  AT THIS CONDITION, THE ELEMENT IN ITS

C      STABLE MODIFICATION OR STRUCTURAL STATE IS ASSIGNED H(298,1)
=
C      0.0 J/MOL.
C
C
C                                 INVERSIONS
C
C   AT AN INVERSION TEMPERATURE AT 1 BAR TOTAL PRESSURE, TWO
STRUCTURAL
C       STATES OF A COMPOUND ARE AT EQUILIBRIUM.  BY DEFINITION,
DELTA
C      G(INVERSION) = 0.0 J/MOL.  BY SPECIFYING THE INVERSION
```

```
C     TEMPERATURE AND THE STRUCTURAL MODIFICATIONS AT EQUILIBRIUM
AT
C     THAT TEMPERATURE, THE PROGRAM OPTIMIZES THE CONSTANTS TO
C     INCLUDE THAT CONSTRAINT ON THE GIBBS ENERGIES OF THE PHASES.
C
C
C                         FUNDAMENTAL CONSTANTS
C
C  THE FUNDAMENTAL CONSTANTS USED IN THIS OPTIMIZATION PROCEEDURE
ARE
C     CONTAINED IN THE "BLOCK DATA" ROUTINE AND GIVEN BELOW.  THEY
WERE
C     TAKEN FROM THE FOLLOWING SOURCE:
C
C  COHEN, E.R.  AND TAYLOR, B.N., 1986, THE 1986 ADJUSTMENT OF THE
C       FUNDAMENTAL PHYSICAL CONSTANTS:  CODATA BULLETIN 63, 32
PAGES.
C      [SEE ALSO MILLS AND OTHERS, 1988, QUANTITIES, UNITS, AND
SYMBOLS
C      IN PHYSICAL CHEMISTRY:  BLACKWELL SCI.  PUBL, OXFORD, 134
PAGES].
C
C     R  =  MOLAR GAS CONSTANT    8.314510 J/(MOL K)
C     F  =  FARADAY CONSTANT      96485.309 COULOMBS/MOL
C     NA =  AVOGADRO CONSTANT     6.0221367*10**23/MOL
C
C
C                                  SUMMARY
C
C  TDM CONTAINS A 25-CONSTANT SET OF PARAMETRIC EQUATIONS FOR THE
C     PROPERTIES OF EACH PHASE IN A CHEMICAL SYSTEM.  THE FUNCTIONS
ARE
C     DERIVED FROM THE EQUATIONS FOR HEAT CAPACITY AND FOR THE
C     COEFFICIENTS OF VOLUME EXPANSION AND OF VOLUME COMPRESSION.
TDM
C     READS A FORMATTED DATA FILE, CONVERTS THE OBSERVATIONS TO
C     STANDARDIZED UNITS, AND FITS THE MODEL FUNCTIONS FOR THE
C      PROPERTIES TO THE DATA FOR THOSE PROPERTIES.  NONLINEAR
FITTING
C      PROCEDURES ARE USED.  WEIGHTING OF THE DATA IS MANDATORY
BECAUSE
C     THE VALUES FOR DIFFERENT PROPERTIES VARIES BY MANY ORDERS OF
C     MAGNITUDE.  TO ACCOMPLISH THE WEIGHTING, THE PRECISION OF THE
C     OBSERVATION SHOULD BE SUPPLIED.  THE PROGRAM THEN CALCULATES
THE
C     WEIGHT FOR EACH OBSERVATION FROM THE PRECISION SUPPLIED FOR
EACH
C     OBSERVATION.
C
C  TDM RETURNS THE RESULTS OF THE LEAST-SQUARES FITTING AS TABLES
OF
C     CONSTANTS FOR EACH PHASE, AS TABLES OF STATISTICAL ANALYSES
OF
C       THE OBSERVED AND CALCULATED VALUES, AND AS A TABLE OF
```

```
INDEPENDENT
C      PARAMETERS, THE DEPENDENT PARAMETER, AND THE CALCULATED
VALUE.
C     THE LATTER FILE IS TO BE USED FOR INPUT TO PLOTTING ROUTINES.
C       THE FITTED CONSTANTS ARE USED BY OTHER PROGRAMS SUCH AS
"RECKON"
C     TO PREPARE TABLES OF RECOMMENDED VALUES FOR PUBLICATION.
C
C
C       PRINTER PLOTS ARE DISABLED WITH THIS VERSION.  REFER TO
STATEMENTS
C        THAT BEGIN WITH "C     CALL PLOT---" OR STATEMENTS THAT
C        BEGIN WITH "C" AND CONTAIN WRITE STATEMENTS TO UNIT 3.
C        --BY HAAS, DECEMBER, 1986.
C
------------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
      CHARACTER*1 IMAGE
      CHARACTER*1 BCD,LABEL
      CHARACTER*1 ALINE,ALINE2,CONT
                        C   H   A   R   A   C   T   E   R   *   8
FILE,FILE01,FILE02,FILE03,FILE04,FILE50,FILE60,FILE07,
     1            FILE09,FILE10,FILE11,FILE12,FILE66
      CHARACTER*8 UNIT,TRUE,ANAME,PHINV,ANOM,NOANOM
      CHARACTER*8 PNAME,TITLE,REF,RECKON,UNITS,YESNO,TYPE,ASTAR
      CHARACTER*12F01,F02,F03,F04,F50,F60,F07,F09,F10,F11,F12,F66
      CHARACTER*23 DATED
      CHARACTER*23 DATE_,DATE2
      CHARACTER*160 LINE,LINE2
      LOGICAL*1 LAMBDA,NOLAM,UNDAMP
      REAL*4XMAX,XMIN,YMAX,YMIN,XI,E,ACOEF,T,TO,AVAL,RELERR,SERR,
     1      SERRSQ,EBAR,STDEV,ERR,AN
C
------------------------------------------------------------------
C      PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C       IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C        DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C        MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C      PARAMETER IP1=   4        ! MAX. NO. OF PHASES IN PROBLEM.
C      PARAMETER IP2=2500        ! MAX. NO. OF OBSERVATIONS.
C      PARAMETER IP3= 250        ! MAX. NO. OF DATA SETS.
C         PARAMETER IP4=    4          ! MAX. NO. OF PHASES PER
OBSERVATION.
C      PARAMETER IP5=IP4+1       ! SPECIAL.  USED IN "PUTPUT".
C        PARAMETER NCPARM=10       ! NO. OF CONSTANTS IN THERMAL
FUNCTIONS.
C       PARAMETER NMPARM=4        ! NO. OF CONSTANTS FOR MAGNETIC
```

```
ANOMALY.
C         PARAMETER NVPARM=8         ! NO. OF CONSTANTS IN VOLUME
FUNCTION.
C        PARAMETER NLPARM=3        ! NO. OF INTEGER CONST. IN LAMBDA
ANOM.
C       PARAMETER NPARM=NCPARM+NMPARM+NVPARM+NLPARM  !TOTAL NO. OF
CONST.
C       PARAMETER IP6=NPARM*IP1 ! MAXINUM NO. OF CONSTANTS.
C        PARAMETER IP7=IP6/1      ! MAXINUM NO. OF CONSTANTS TO BE
FIT.
C       PARAMETER IP8=IP7*(IP7+3)/2 ! SPECIAL.  USED IN "MINV".
C       PARAMETER IP9=28          ! NO. OF LABELS FOR DATA TYPES.
C      PARAMETER IP10=2         ! MAX. NO. OF TRANSITIONS IN SERIES.
C       PARAMETER IP11=IP10+1    ! MAX. NO. OF PHASES IN TRANSITION
SERIES.
C
C
-----------------------------------------------------------------
                              D   I   M   E   N   S   I   O   N
AVAL(7),SERR(3),SERRSQ(3),EBAR(3),STDEV(3),IMAGE(5000),
     1  XI(1),E(1),PHINV(6),VAL(7),IFMIN(IP1),TRUE(2),DATED(IP1)
      DIMENSION NOANOM(2)
      DIMENSION TCTK(2)
      DIMENSION LINE(IP3),ALINE(160,IP3),ALINE2(160)
      DIMENSION COEF(IP4,IP3),TINV(IP4,IP3,IP10),NPHASE(IP3),
                1
IKOUNT(IP3),IGO(IP3),ISTATE(IP4,IP3),INSTAT(IP4,IP3),
     2         INVPH(IP4,IP3,IP11),INVSC(IP4,IP3),ISPECL(IP4,IP3),
     3           IPHASE(IP4,IP3),NINVER(IP4,IP3)
                              D   I   M   E   N   S   I   O   N
X(NX,IP2),P(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1          ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION ERRP(IP6),IHOLD(IP1),ITEK(4)
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION DYDC(NCPARM),DHDC(NCPARM),DGDC(NCPARM),DLYDC(2),
     1           DLHDC(2),DLGDC(2)
      DIMENSION AA(IP6)
      DIMENSION LAMBDA(IP1),NOLAM(IP4,IP3)
      DIMENSION PNAME(IP1),TITLE(10),REF(20,IP3),UNITS(4),YESNO(2),
     1           TYPE(IP9),LABEL(50)
      COMMON /EARTH/ COEF,TINV,NPHASE,IKOUNT,IGO,ISTATE,INSTAT,
     1                INVPH,INVSC,ISPECL,IPHASE,NINVER,NSETS,LISTP
      COMMON /AIR/ X,P,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1              ISING,ISTOP,IL,JDF,ION
                       C   O   M   M   O   N      /   F   I   R   E   /
ERRP,IWRITE,ICY,IICY,IREDO,IREG,NHOLD,IHOLD,ITEK,
     1               IDUMP
                      C   O   M   M   O   N      /   W   A   T   E   R   /
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1                STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /TIME_/ DATE_
      COMMON /SPACE/ DYDC,DHDC,DGDC,DLYDC,DLHDC,DLGDC,SC,T2,PT
      COMMON /MAN/ AA
      COMMON /AETHER/ LAMBDA,NOLAM,UNDAMP
```

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      COMMON /OCEAN/ RJ,RC,FJ,FC
      COMMON /HOTAIR/ PNAME,TITLE,REF,UNITS,RECKON,YESNO,ASTAR,
     1                TYPE,LABEL,BCD
      EQUIVALENCE (FILE01,F01),(FILE02,F02),(FILE03,F03),
     1            (FILE04,F04),(FILE50,F50),(FILE60,F60),
     2            (FILE07,F07),(FILE09,F09),(FILE10,F10),
     3            (FILE11,F11),(FILE12,F12),(FILE66,F66)
      EQUIVALENCE (LINE(1),REF(1,1))
      EQUIVALENCE (LINE(1),ALINE(1,1))
      EQUIVALENCE (LINE2,ALINE2(1))
      DATA F01/'        .TMP'/,F02/'        .MAT'/,
     1     F03/'        .SUM'/,F04/'        .TBL'/,
     2     F50/'        .DAT'/,F60/'        .REG'/,
     3     F07/'        .CON'/,F09/'        .PT1'/,
     4     F10/'        .PT2'/,F11/'        .PT3'/,
     5     F12/'        .HAV'/,F66/'        .DMP'/
      DATA NOANOM/'NOLAM','nolam'/
      DATA CONT/'>'/
      DATA TRUE/'reckon  ','RECKON  '/
      DATA TCTK/25.D0,298.15D0/
C
-----------------------------------------------------------------
C     READ IN AND STORE INPUT DATA--
C          DATE_ -- TODAY'S DATE
C                     GET TODAY'S DATE-TIME FROM THE SYSTEM.
C           FILE -- A USER-SUPPLIED IMAGE TO IDENTIFY THE PROBLEM
BEING
C                     SOLVED.
C          NREG -- NUMBER OF SEPARATE PROBLEMS IN THE DATA SET
C
-----------------------------------------------------------------
      WRITE (6,5599)
 5599 FORMAT(' TYPE IN AN 8-CHARACTER STRING GIVING THE DATA-FILE
NAME.'
     1/'  PAD THE NAME TO 8 CHARACTERS AND DO NOT INCLUDE BLANKS IN
'
     2/'  THE DATA-FILE NAME:  ^G^G^G')
      READ (5,5600) FILE
      FILE01=FILE
      FILE02=FILE
      FILE03=FILE
      FILE04=FILE
      FILE50=FILE
      FILE60=FILE
      FILE07=FILE
      FILE09=FILE
      FILE10=FILE
      FILE11=FILE
      FILE12=FILE
      FILE66=FILE
      OPEN (UNIT=50,FILE=F50,
     1     ACCESS="SEQUENTIAL",
     2     FORM="FORMATTED",
     3     STATUS="OLD",
```

```
     4      ACTION="READ")
      OPEN (UNIT=1,FILE=F01,
     1      ACCESS="SEQUENTIAL",
     2      FORM="FORMATTED",
     3      STATUS="UNKNOWN",POSITION="REWIND",
     4      ACTION="WRITE")
      OPEN (UNIT=60,FILE=F60,
     1      ACCESS="SEQUENTIAL",
     2      FORM="FORMATTED",
     3      STATUS="UNKNOWN",POSITION="REWIND",
     4      ACTION="WRITE")
      OPEN (UNIT=2,FILE=F02,
     1      ACCESS="SEQUENTIAL",
     2      FORM="FORMATTED",
     3      STATUS="UNKNOWN",POSITION="REWIND",
     4      ACTION="WRITE")
      OPEN (UNIT=7,FILE=F07,
     1      ACCESS="SEQUENTIAL",
     2      FORM="FORMATTED",
     3      STATUS="UNKNOWN",POSITION="REWIND",
     4      ACTION="WRITE")
      CALL ERRORS
      CALL TIMELY(DATE_)
      READ (50,5800) NREG
      DO 5400 IREG=1,NREG
C
----------------------------------------------------------------
C     INITIALIZE CONSTANTS
C     WRITE DATE AND TIME FOR BEGINNING OF RUN.
C
----------------------------------------------------------------
      SSQRSG=ZERO
      IICY=0
      KOUNT=0
      IWRITE=1
      WRITE (1,6600) DATE_
C
----------------------------------------------------------------
C     READ IN AND STORE --
C        TITLE -- TITLE FOR CORRELATION
C        IDO -- 1 FOR REGRESSION AND ERROR PLOTS
C           2 FOR REGRESSION ONLY
C           3 FOR ERROR PLOTS ONLY
C        NC -- NUMBER OF CYCLES. GENERALLY 2 ARE SUFFICIENT.
C           THE SUBROUTINE TEST WILL TERMINATE THE REGRESSION IF
THE
C           RELATIVE CHANGE IN SUCCESSIVE PARAMETERS IS LESS THAN
C           1.0D-8.
C        IW -- 0 FOR WEIGHTED DATA
C           1 FOR UNWEIGHTED DATA
C        IL -- 0 FOR CALCULATED RESULTS AT PLOT TIME ONLY
C           1 FOR CALCULATED RESULTS WITH EACH CYCLE
C        IFMOUT -- PRINT FORMAT FOR OUTPUT OF PARAMETERS--
C           0 GIVES PARAMETERS IN 6D12.5 FORMAT
```

```
C           1 GIVES PARAMETERS IN 6A8 FORMAT.
C             UNIT -- UNITS USED IN CALCULATIONS ('JOULES' OR
'CALORIES')
C           THE DEFAULT IS JOULES.
C        RECKON -- PRINTED OUTPUT NEEDED FOR PROGRAM 'RECKON'
C           'RECKON  ' PRODUCES PRINT.
C           'NORECKON' OR BLANK PRODUCES NO PRINT.
C        ITEK --  PRINTS A FILE CONTAINING THE FOLLOWING
C           "JSET;X(1,I),X(2,I),X(3,I),X(4,I),YO(I),YC"
C           THE FILE IS FOR USE WITH PLOTTERS AND CONTAINS THE
C           SEMICOLON AND COMMAS TO SEPARATE THE DATA.
C        LISTP -- NUMBER OF PHASES IN CORRELATION
C        ICY -- NUMBER OF STEPS IN STEP-BACKWARD ELIMINATION.
C           DEFAULT IS 0.
C        NHOLD -- NUMBER OF PARAMETERS TO BE KEPT WITHIN THE
C           REGRESSION EVEN THOUGH 'TEST' WILL INDICATE THEY ARE
C           NOT SIGNIFICANT.  THIS IS IMPORTANT FOR THE
C           TWO CONSTANTS OF INTEGRATION, a(9) AND a(10) FOR EACH
C           PHASE.
C        IDAMP -- SET TO 0 IF YOU WANT TO CAUSE UNDAMPING OF A
C           REFINEMENT DURING SUCCESSIVE CYCLES.  NOT NEEDED IF
C           DAMPING IS NOT USED.
C           SET TO 1 IF THE SAME DAMPING IS TO BE USED THRU
C           THE REFINEMENT.
C        PNAME(LISTP) -- 8-CHARACTER LABEL FOR EACH PHASE IN
C           CORRELATION.
C        NSETS -- NUMBER OF DATA SETS IN CORRELATION
C
-----------------------------------------------------------------
      READ (50,5600) (TITLE(I),I=1,10)
                                             R      E      A      D
(50,10000)IDO,NC,IW,IL,IFMOUT,UNIT,RECKON,(ITEK(I),I=1,4)
      UNDAMP=.TRUE.
      READ (50,5700) LISTP,ICY,NHOLD,IDAMP
      IF(IDAMP.EQ.1)  UNDAMP=.FALSE.
      READ (50,5600) (PNAME(M),M=1,LISTP)
      READ (50,5700) NSETS
      WRITE (1,6700) (TITLE(I),I=1,10)
      WRITE (1,6800) (PNAME(M),M=1,LISTP)
      WRITE (1,6500)
      WRITE (1,6900) (TITLE(I),I=1,10),DATE_
      WRITE (1,7000)
      WRITE (2,5600) (TITLE(I),I=1,10)
      IF((RECKON.EQ.TRUE(1)).OR.(RECKON.EQ.TRUE(2)))
     1     GO TO 1
      WRITE (2,5700) LISTP
      WRITE (2,5600) (PNAME(M),M=1,LISTP)
    1 CONTINUE
      WRITE (7,5600) (TITLE(I),I=1,10)
      WRITE (7,5700) LISTP
      WRITE (7,5600) (PNAME(M),M=1,LISTP)
      DO 3 I=1,4
      IF(UNITS(I).EQ.UNIT)  GO TO 4
    3 CONTINUE
```

```
      I=1
    4 CONTINUE
      GO TO (5,5,6,6),I
C
------------------------------------------------------------------------
C     ENERGY UNITS ARE IN JOULES.  (DEFAULT IF NOT SPECIFIED.)
C
------------------------------------------------------------------------
    5 CONTINUE
      R=RJ
      F=FJ
      GO TO 7
C
------------------------------------------------------------------------
C     ENERGY UNITS ARE IN CALORIES.
C
------------------------------------------------------------------------
    6 CONTINUE
      R=RC
      F=FC
    7 CONTINUE
C
------------------------------------------------------------------------
C     READ IN AND STORE INPUT DATA FOR EACH DATA SET --
C         REF (IP4,J) -- REFERENCE FOR 'J'TH DATA SET (DATA SET
C            IDENTIFICATION).  THE VARIABLE "LINE(J)" IS
C            EQUIVALENT TO THE VARIABLE "REF(?,J)".
C            FOR CONTINUATION OF THE REFERENCE INFORMATION OR FOR
C                ADDITIONAL NOTES RELATED TO A DATA SET AND ITS
CONVERSION
C           FOR INPUT, ENTER ">" AS THE LAST CHARACTER ON EACH LINE

C              EXCEPT THE FINAL LINE OF THE REFERENCE INFORMATION.
THE
C             ADDITIONAL LINES ARE NOT USED IN THE PROGRAM BUT ARE
NEEDED
C            SO THAT THE USER KNOWS HOW A DATA SET WAS PROCESSED.
C         NPHASE(J) -- NUMBER OF PHASES IN REACTION, SET TO 1 WHEN
C            DATA FOR ONE PHASE ONLY.
C         IKOUNT(J) -- NUMBER OF OBSERVATIONS IN DATA SET
C         IGO(J) -- DATA TYPE:
C            IGO(J)     DATA TYPE OR FUNCTION
C               1       CP(T,1) AND DELTA CP(T,1)
C              1      CP(T,1)-CP(TO,1); ISPECL(L,J)=-1 FOR PHASE AT
TO.
C               2       S(T,1) AND DELTA S(T,1)
C              2      S(T,1)-S(TO,1); ISPECL(L,J) = -1 FOR PHASE AT
TO.
C               3       H(T,1) AND DELTA H(T,1)
C              3      HEAT OF SOLUTION WHERE PHASE AT A TEMPERATURE
C                          OTHER THAN THE REACTION TEMPERATURE.
C               4       G(T,1) AND DELTA G(T,1)
C               5       LOG K, EQUILIBRIUM CONSTANT
C               6       E, ELECTROCHEMICAL POTENTIAL
```

```
C                  7       H(T,1)-H(TR,1), INCREMENTAL (OR RELATIVE)
ENTHALPY
C                 8       GEF(T,1) AND DELTA GEF(T,1)
C                 9       CV(T,1)
C                10       T(CRIT) = FUNCTION OF PRESSURE
C                11       V(T,P), MOLAR VOLUME.
C                12       V(T,P), CELL VOLUME.
C               13       V-VO, VOLUME RELATIVE TO A REFERENCE VOLUME.
C                14       V/VO, REDUCED VOLUME.
C                15       ALPHA, CUBIC EXPANSION COEFFICIENT.
C                16       (V-VO)/VO AT CONSTANT PRESSURE.
C                17       (V-VO)/[VO*(T-TO)] AT CONSTANT PRESSURE.
C                18       KAPPA-T(T,P), ISOTHERMAL COMPRESSIBILITY.
C                19       B-T(T,P), ISOTHERMAL BULK MODULUS.
C                20       (V-VO)/VO AT CONSTANT TEMPERATURE.
C                21       (V-VO)/[VO*(P-PO)] AT CONSTANT TEMPERATURE.
C                  22       G(T,P) AND DELTA G(T,P), GIBBS ENERGY AT
ELEVATED
C                           PRESSURE.
C                23       KAPPA-S(T,1), ISENTROPIC COMPRESSIBILITY.
C                24       B-S(T,1), ISENTROPIC BULK MODULUS.
C                     25          GRUENEISEN CONSTANT, GAMMA (to be
programmed).
C                26       dP/dT AT P = 0.
C               27-99     UNASSIGNED.  TO BE USED TO EXPAND THE ABOVE
LIST.
C            FOR ANY DATA NOT INCLUDED IN THE TYPES GIVEN ABOVE, SET
C                IGO(J) TO ANY INTEGER GREATER THAN 100.  SUPPLY
C                    THE SUBROUTINE  UNIQUE TO CALCULATE YC (AND
DERIVATIVES
C                DC(I) IF JDF (OR JDFLAG) = ZERO) FROM THE CURRENT
VALUES
C                OF THE PARAMETERS.  IF MORE THAN ONE TYPE OF DATA
ARE TO
C                BE CONSIDERED, THEY ARE KEYED BY DIFFERENT VALUES
C                OF IGO(J).
C          ITFACT -- THE VALUES IS 1 IF TEMPERATURE IS IN KELVINS,
C             0 IF THE TEMPERATURE IS IN CENTIGRADE DEGREES.
C          IYFACT -- PROGRAM IS SET FOR UNITS IN JOULES OR CALORIES
AS
C               SPECIFIED, VOLTS, OR LOG(10)K IN MOLAL (OR MOLAL)
UNITS.
C             IF SO, SET IYFACT TO 1
C             IF NOT, SET IYFACT TO 0. PROGRAM MULTIPLIES YO(I) AND
C             SIGYO(I)BY PARA TO BE READ LATER.
C          ISIG -- 0 IF WEIGHTS ARE RELATIVE.
C             1 IF WEIGHTS ARE ABSOLUTE.
C             (ABSOLUTE WEIGHTS ARE USED IN CALCULATIONS.)
C         I6X -- SET TO 1 IF 3 OR MORE INDEPENDENT PARAMETERS ARE TO
BE
C             READ.  PLACE X(3,I), X(4,I), PFACT, X(5,I), X(6,I)
C             AND XXFACT IN 6D12.5 FORMAT IN THAT ORDER.
C               SET TO 0 FOR WHEN X(1,I) AND X(2,I) ARE THE ONLY
INDEPENDENT
```

```
C            PARAMETERS TO BE SUPPLIED FOR THE DATA SET.
C        IPFACT-- THE VALUE IS 1 IF THE PRESSURES ARE IN BARS.  THE
C            VALUE IS 0 IF OTHER UNITS ARE USED.
C         IXFACT -- THE VALUE IS 1 IF THE UNITS ARE STANDARD.  THE
C            VALUE IS 0 IF THE X(5,I) AND X(6,I) ARE TO BE
C            MODIFIED.
C
-------------------------------------------------------------------
      DO 1800 J=1,NSETS
      IQ=80
      READ (50,5602) LINE(J)
      IF(ALINE(IQ,J).NE.CONT)  GO TO 20
   10 CONTINUE
      READ (50,5602) LINE2
      IF(ALINE2(IQ).EQ.CONT)  GO TO 10
   20 CONTINUE
      WRITE (1,7100)
      WRITE (1,7200) ASTAR
      WRITE (1,7100)
      WRITE (1,7300) J,(REF(I,J),I=1,15)
                    READ (50,5700)
NPHASE(J),IKOUNT(J),IGO(J),ITFACT,IYFACT,ISIG,I6X,
     1              IPFACT,IXFACT
      IGOES=IGO(J)
      IF(IGOES.GT.28)  IGOES=28
      WRITE (1,7400) NPHASE(J),IKOUNT(J),TYPE(IGOES)
      NPHAS=NPHASE(J)
C
-------------------------------------------------------------------
C     FOR EACH DATA SET, READ AND STORE FOR ONE PHASE AT A TIME,
C        ANAME -- 8-CHARACTER PHASE LABEL. MUST BE THE SAME AS
C           GIVEN IN "PNAME(LISTP)".  IF NOT FOUND, PRINT ERROR
MESSAGE.
C        COEF(I,J) -- COEFFICIENT IN REACTION (+1.0D0 IF NOT
C           REACTION).
C        ISPECL(I,J) -- FLAG USED TO ALLOW FOR SPECIAL CASES IN
C           HEATS OF SOLUTION, CP(T,1)-CP(To,1), S(T,1)-S(To,1),
C            ETC., AND WHERE CELL VOLUMES ARE TO BE CONVERTED TO
MOLAR
C           VOLUMES.
C        ANOM(I,J) --  INSERT "NOLAM" IF THE CONTRIBUTION TO THE
C           THERMAL FUNCTION IS TO BE IGNORED FOR THIS DATA SET.
C            ISTATE(I,J) -- FOR ELEMENTS IN LOWEST TEMPERATURE
MODIFICA-
C           TION, SET TO 1.
C           FOR COMPOUNDS AND ELEMENTS IN HIGHER TEMPERATURE
C           MODIFICATIONS, SET TO 0.
C        NINVER (I,J) -- NUMBER OF INVERSIONS (EQUALS NUMBER OF
C               MODIFICATIONS BEING CONSIDERED IN THE INVERSION
SEQUENCE
C           FOR COMPONENT.)
C
-------------------------------------------------------------------
      DO 700 I=1,NPHAS
```

```
      READ (50,6000) ANAME,COEF(I,J),ISPECL(I,J),ANOM,ISTATE(I,J),
     1               NINVER(I,J)
C
-----------------------------------------------------------------
C     LOCATE "ANAME" IN LIST "PNAME(LISTP)" AND ASIGN THE INDEX TO
C       IPHASE(I,J).
C
-----------------------------------------------------------------
      DO 100 K=1,LISTP
      IF (ANAME.EQ.PNAME(K)) GO TO 200
  100 CONTINUE
      GO TO 5200
  200 IPHASE(I,J)=K
      NOYES=(ISTATE(I,J)+3)/2
      ACOEF=COEF(I,J)
                    WRITE (1,7500)
PNAME(IPHASE(I,J)),ACOEF,YESNO(NOYES),NINVER(I,J)
      NOLAM(I,J)=.FALSE.
       IF((ANOM.EQ.NOANOM(1)).OR.(ANOM.EQ.NOANOM(2)))
NOLAM(I,J)=.TRUE.
      IF (NINVER(I,J).EQ.0) GO TO 700
C
-----------------------------------------------------------------
C     IF "(NINVER(I,J).GT.0)" READ AND STORE,
C        INSTAT(I,J) -- FOR ELEMENTS,ASIGN 1
C           FOR COMPOUNDS, ASIGN 0
C        INVSC(I,J) -- IF UPON INVERSION THERE IS A STOICHIOMETRY
C               CHANGE (EG-- 2 FECL3 = FE2CL6), THEN FIND THE
APPROPRIATE
C           REACTANT COEFFFICIENT (HERE '2') IN THE VECTOR STCOEF
AND
C           ENTER HERE.  DEFAULT GIVES A COEFFICIENT OF '1'.
C        TINV(NINVER(I,J)) -- INVERSION TEMPERATURES, KELVINS
C        PHINV(NINVER(I,J)+1) -- PHASE NAME FOR ALL MODIFICATIONS,
C           BEGINNING WITH LOWEST TEMPERATURE MODIFICATION FIRST.
NAME
C           MUST CONFORM WITH THE NAMES IN PNAME(LISTP).
C
-----------------------------------------------------------------
      KINVER=NINVER(I,J)
      READ (50,6100) (TINV(I,J,K),K=1,KINVER)
      KINVER=KINVER+1
      READ (50,6200) INSTAT(I,J),INVSC(I,J),(PHINV(K),K=1,KINVER)
      IF (INVSC(I,J).EQ.0) INVSC(I,J)=1
C
-----------------------------------------------------------------
C      LOCATE "PHINV(NINVER(I,J)+1)" IN LIST "PNAME(LISTP)" AND
ASIGN THE
C        INDEX TO "INVPH(I,J)".
C
-----------------------------------------------------------------
      DO 500 K=1,KINVER
      DO 300 L=1,LISTP
      IF (PHINV(K).EQ.PNAME(L)) GO TO 400
```

```
  300 CONTINUE
      GO TO 5200
  400 INVPH(I,J,K)=L
  500 CONTINUE
      KINVER=KINVER-1
      WRITE (1,7600)
      ACOEF=1.0
      DO 600 K=1,KINVER
      IF (K.EQ.KINVER) ACOEF=STCOEF(INVSC(I,J))
      T=TINV(I,J,K)
                      WRITE (1,7700)
ACOEF,PNAME(INVPH(I,J,K)),PNAME(INVPH(I,J,K+1)),T
  600 CONTINUE
      IF (INSTAT(I,J).EQ.1) WRITE (1,7800) PNAME(INVPH(I,J,1))
  700 CONTINUE
C
-------------------------------------------------------------------
C       INITIALIZE "KO", "KOUNT" AND "IKOUNT(I)".  AFTER DATA IS
STORED,
C         "IKOUNT(I)" CONTAINS THE LOCATION OF THE LAST ITEM IN THE
C         'J'TH DATA SET.
C
-------------------------------------------------------------------
      KO=KOUNT+1
      KOUNT=KOUNT+IKOUNT(J)
      IKOUNT(J)=KOUNT
      WRITE (1,7900)
      IGOES=IGO(J)
      IF(IGOES.GT.28)  IGOES=8
      WRITE (1,8000) TYPE(IGOES)
C
-------------------------------------------------------------------
C     READ AND STORE THE DATA IN THE 'J'TH DATA SET,
C         X(1,I) -- TEMPERATURE (SEE TFACT BELOW)
C         TFACT -- 0.0D0 IF TEMPERATURE IN KELVINS
C            273.15D0 IF TEMPERATURE IN CELSIUS DEGREES
C         YO(I)  -- DEPENDANT OBSERVATION
C         PARA -- CONVERSION FACTOR TO CONVERT DATA TO CALORIES OR
C            VOLTS (1.D3 FOR DATA IN KILOCALORIES, 1.0D-3 FOR DATA
IN
C           MILLIVOLTS, --OR THE APPROPRIATE CONVERSION FACTOR FOR
DATA
C            IN JOUES, BUT/LB, QUART*STONES/ACRE, ETC.).
C        SIGYO(I)  -- SEE PROGRAM DESCRIPTION FOR ASIGNING WEIGHTS.
C        X(2,I) -- FOR DATA TYPES (IGO(J)) FROM 1 THRU 6, GENERALLY
SET
C               X(2,I) = ZERO.
C            FOR RELATIVE HEAT CONTENT DATA, X(2,I) IS THE BASE
C               TEMPERATURE.  DEFAULT IS TREF IN THE BLOCKDATA
C               ROUTINE.
C            FOR DATA TYPES TO BE PROGRAMMED BY THE USER,
C               X(2,I) IS AN OPTIONAL SECOND INDEPENDENT
C               VARIABLE.
C           FOR DATA WHERE "ISPECL(I,J)" IS -1, X(2,I) IS THE BASE
```

```
C              TEMPERATURE, TO.  EXAMPLE:  S(T,1)-S(TO,1).
C       X(3,I) -- INDEPENDENT PARAMETER #3.  FOR ALL PREPROGRAMMED
C           FUNCTIONS, THIS IS THE PRESSURE OF THE OBSERVATION.
C       X(4,I) -- INDEPENDENT PARAMETER #4.  FOR ALL PREPROGRAMMED
C           FUNCTIONS, THIS IS THE REFERENCE PRESSURE.  THE
C           DEFAULT IS GIVEN BY PREF IN THE BOCKDATA SUBROUTINE.
C        PFACT  -- CONVERSION FACTOR FOR UNITS GIVEN TO BARS.
C         X(5,I) -- INDEPENDENT PARAMETER #5.  FOR CELL VOLUMES,
"z", THE
C             NUMBER OF FORMULA UNITS PER UNIT CELL, IS INSERTED
HERE.
C           THIS ALLOWS THE OPTION TO FIT THE CELL VOLUMES OR THE
MOLAR
C           VOLUMES.
C        X(6,I) -- INDEPENDENT PARAMETER #6.  UNASSIGNED.
C        XFACT  -- CONVERSION FACTOR FOR UNITS.  UNASSIGNED.
C
-----------------------------------------------------------------
      DO 1700 I=KO,KOUNT
      IF(I6X.EQ.1)  GO TO 800
      READ (50,6100) X(1,I),TFACT,YO(I),YFACT,SIGYO(I),X(2,I)
      DO 750 K=3,6
      X(K,I)=ZERO
  750 CONTINUE
      PFACT=ZERO
      XFACT=ZERO
      GO TO 900
  800 CONTINUE
      READ (50,6100)X(1,I),TFACT,YO(I),YFACT,SIGYO(I),X(2,I),
     1             X(3,I),X(4,I),PFACT,X(5,I),X(6,I),XFACT
  900 CONTINUE
      IF    ((IW.EQ.0).AND.(SIGYO(I).EQ.0.0D0).AND.(ISIG.EQ.0))
SIGYO(I)=
     1      1.0D3*YO(I)
      IF(X(2,I).EQ.0.D0)  X(2,I)=TCTK(1+ITFACT)
      IF (ITFACT.EQ.1) GO TO 1000
C
-----------------------------------------------------------------
C     IF ITFACT = 0,     X(1,I) = X(1,I) + TFACT
C
-----------------------------------------------------------------
      X(1,I)=X(1,I)+TFACT
      X(2,I)=X(2,I)+TFACT
 1000 CONTINUE
      IF (IYFACT.EQ.1) GO TO 1100
      IF(IYFACT.EQ.-1)  GO TO 1050
C
-----------------------------------------------------------------
C     IF IYFACT = 0,     YO(I) = YO(I)*YFACT
C
-----------------------------------------------------------------
      YO(I)=YO(I)*YFACT
      GO TO 1100
C
```

```
-----------------------------------------------------------------
C     CONVERTING FROM CELL VOLUME TO MOLAR VOLUME,
C     IF IYFACT.EQ.-1      YO(I) = YO(I)*A/YFACT
C        WHERE A = (AVAGADRO'S NUMBER)/10**24  AND
C        YFACT = Z, THE NUMBER OF FORMULA UNITS IN THE UNIT CELL.
C
C       YO(I) WAS THE VOLUME OF CRYSTALLOGRAPHIC UNIT CELL IN
ANGSTROMS.
C     THE NEW YO(I) IS THE MOLAR VOLUME.
C
-----------------------------------------------------------------
 1050 CONTINUE
      YO(I)=YO(I)*A/YFACT
 1100 CONTINUE
      IF (IW.EQ.1) GO TO 1300
      IF (ISIG.EQ.1) GO TO 1200
C
-----------------------------------------------------------------
C     IF ISIG = 0,        SIGYO(I)= DABS (YO(I))*SIGYO(I)
C
-----------------------------------------------------------------
      SIGYO(I)=DABS(SIGYO(I)*YO(I))
      GO TO 1400
 1200 CONTINUE
C
-----------------------------------------------------------------
C     IF IYFACT = 0,      SIGYO(I)=SIGYO(I)*YFACT
C
-----------------------------------------------------------------
      IF(IYFACT.EQ.0)  SIGYO(I)=DABS(SIGYO(I)*YFACT)
C
-----------------------------------------------------------------
C    CONVERTING FOR ERROR IN CELL VOLUME TO ERROR IN MOLAR VOLUME,
C     IF IYFACT = -1,     SIGYO(I) = DABS(SIGYO(I)*A/YFACT)
C
-----------------------------------------------------------------
      IF(IYFACT.EQ.-1)  SIGYO(I)=DABS(SIGYO(I)*A/YFACT)
      GO TO 1400
 1300 CONTINUE
      SIGYO(I)=DABS(YO(I)*1.0D-2)
 1400 CONTINUE
      IF (SIGYO(I).EQ.0.0D0) SIGYO(I)=1.0D3*YO(I)
      IF (SIGYO(I).EQ.0.0D0)  SIGYO(I)=1.0d15
      IF(I6X.EQ.0)  GO TO 1475
C
-----------------------------------------------------------------
C     IF IPFACT = 0,     X(3,I) = X(3,I)*PFACT  AND
C                       X(4,I) = X(4,I)*PFACT
C
-----------------------------------------------------------------
      IF(IPFACT.EQ.1)  GO TO 1450
      X(3,I)=X(3,I)*PFACT
      X(4,I)=X(4,I)*PFACT
 1450 CONTINUE
```

```
C
------------------------------------------------------------------
C     IF IXFACT = 0,     X(5,I) = X(5,I)*XFACT  AND
C                        X(6,I) = X(6,I)*XFACT
C
------------------------------------------------------------------
      IF(IXFACT.EQ.1)  GO TO 1475
      X(5,I)=X(5,I)*XFACT
      X(6,I)=X(6,I)*XFACT
 1475 CONTINUE
      T=X(1,I)
      TO=X(2,I)
      IF (TO.NE.0.0) GO TO 1500
      WRITE (1,8100) I,T,YO(I),SIGYO(I)
      GO TO 1600
 1500 CONTINUE
      WRITE (1,8200) I,T,TO,YO(I),SIGYO(I)
 1600 CONTINUE
      SSQRSG=SSQRSG+(1.D0/SIGYO(I))**2
 1700 CONTINUE
 1800 CONTINUE
      FKOUNT=DBLE(FLOAT(KOUNT))
      DO 1900 I=1,KOUNT
      SIGYON(I)=SIGYO(I)*DSQRT(SSQRSG/FKOUNT)
 1900 CONTINUE
C
------------------------------------------------------------------
C     THE DATA HAS NOW BEEN STORED. INITIALIZE CONSTANTS NEEDED FOR
C        ORGLS.
C
------------------------------------------------------------------
      NO=KOUNT
      NP=LISTP*NPARM
      IW=0
C
------------------------------------------------------------------
C     READ AND STORE,
C        IFMIN -- INPUT FORMAT FOR P(LISTP*NPARM)
C           0 INDICATES (6D12.5/D12.5)
C           1 INDICATES (7A8)
C           THE LATTER FORMAT HAS NO ROUNDOFF IN DATA TRANSFER.
C        P(LISTP*6)  -- TRIAL PARAMETERS. IF VARIED, MAY BE 0.0D0.
C            IF NOT VAIRED, 0.0D0 OR A PREDETERMINED VALUE MAY BE
USED.
C        LAMBDA(LISTP) -- LOGICAL ARGUMENT TO SPECIFY WHETHER
C           CP FUNCTION FOR PHASE HAS LAMBDA ANOMALY.
C        ION(LISTP) -- FLAG WHICH INDICATES THE SPECIES IS A
C          REFERENCE ELEMENT (1), A COMPOUND (0), OR AN ION (-1).
C        KI(LISTP*6)   -- 0 IF PARAMETER IS HELD CONSTANT.
C           1 IF PARAMETER IS TO BE VARIED
C           KI(I) MAY ALSO BE SET TO AN INTEGER RANGING FROM 1 TO
9.
C           IF SET TO AN INTEGER GREATHER THAN 1, DAMPING OF THE
C          REFINEMENT WILL OCCUR.  REFER TO INTRODUCTORY NOTES FOR
```

```
C            THE DAMPING FACTORS ASSOCIATED WITH THE INTEGERS 2
THROUGH 9.
C        IHOLD -- INDICES OF PARAMETERS IN P(LISTP*7) WHICH ARE
C           FORCED TO STAY IN REGRESSION DESPITE DETERMINATION IN
C           "TEST" THAT THESE PARAMETERS MAY BE NON-SIGNIFICANT.
C
-----------------------------------------------------------------------
      READ (50,6300) (IFMIN(I),I=1,LISTP)
      DO 2200 I=1,LISTP
      JO=1+NPARM*(I-1)
      JN=JO+NPARM-1
      IF (IFMIN(I).EQ.1) GO TO 2000
      READ (50,6110) (P(J),J=JO,JN),LAMBDA(I),ION(I),DATED(I)
      GO TO 2100
 2000 CONTINUE
      READ (50,5610) (P(J),J=JO,JN),LAMBDA(I),ION(I),DATED(I)
 2100 CONTINUE
      DO 2200 J=JO,JN
      AA(J)=P(J)
 2200 CONTINUE
      READ (50,6310) (KI(I),I=1,NP)
      IF (NHOLD.NE.0) READ (50,5700) (IHOLD(I),I=1,NHOLD)
C
-----------------------------------------------------------------------
C     CLOSE AND DELETE UNIT 1.  WHEN THE INPUT FILE HAS BEEN READ,
C          THIS FILE IS OF NO FURTHER USE.  RELEASE THE SPACE TO
OTHERS.
C
-----------------------------------------------------------------------
      CLOSE (UNIT=1,STATUS='DELETE')
C
-----------------------------------------------------------------------
C     BYPASS REGRESSION IF IDO IS 3.
C
-----------------------------------------------------------------------
      IF (IDO.EQ.3) GO TO 2700
      IDUMP=60
 2300 CONTINUE
      NV=0
      DO 2400 K=1,NP
      IF (KI(K).EQ.0) GO TO 2400
      NV=NV+1
 2400 CONTINUE
      JDF=0
C
-----------------------------------------------------------------------
C     RESET JDF (I.E. JDFLAG) TO "1" IF NC = 0.
C     THEN ENTER ORGLS AND REFINE PARAMETERS.
C
-----------------------------------------------------------------------
      IF(NC.EQ.0)  JDF=1
      CALL TIMELY(DATE2)
      WRITE (6,10600)DATE2
      OPEN (UNIT=9,FILE=F09,
```

```
     1     ACCESS="SEQUENTIAL",
     2     FORM="FORMATTED",
     3     STATUS="UNKNOWN",POSITION="REWIND",
     4     ACTION="WRITE")
      OPEN (UNIT=66,FILE=F66,
     1     ACCESS="SEQUENTIAL",
     2     FORM="FORMATTED",
     3     STATUS="UNKNOWN",POSITION="REWIND",
     4     ACTION="WRITE")
      CALL ORGLS
      CALL TIMELY (DATE2)
      WRITE (6,10700)DATE2
      IF (ISING.NE.0) GO TO 2700
      IF(NC.EQ.0)  GO TO 2650
C
----------------------------------------------------------------
C     PRINT REFINED PARAMETERS, ONE PHASE AT A TIME AND INCLUDE
C         THE PHASE NAME ON THE IMAGE WITH THE RELATED PARAMETERS.
C          PLACE THE DATE THE PARAMETERS WERE LAST MODIFIED ON THE
C             LAST IMAGE FOR EACH PHASE.  IF THE CONSTANTS WERE
MODIFIED
C                IN THIS CYCLE, THEN USE THE CURENT DATE-TIME
INFORMATION.
C
----------------------------------------------------------------
      DO 2600 I=1,LISTP
      JO=1+NPARM*(I-1)
      IF (IFMOUT.EQ.1) GO TO 2500
      JN=JO+5
      DO 2410 J=JO,JN
      IF(KI(J).EQ.0)  GO TO 2410
      DATED(I)=DATE_
      IPASS=1
      GO TO 2420
 2410 CONTINUE
 2420 CONTINUE
      WRITE (7,9600) (P(J),J=JO,JN),PNAME(I)
      JO=JN+1
      JN=JN+6
      IF(IPASS.EQ.1)  GO TO 2440
      DO 2430 J=JO,JN
      IF(KI(J).EQ.0)  GO TO 2430
      DATED(I)=DATE_
      IPASS=1
      GO TO 2440
 2430 CONTINUE
 2440 CONTINUE
      WRITE (7,9600) (P(J),J=JO,JN),PNAME(I)
      JO=JN+1
      JN=JN+6
      IF(IPASS.EQ.1)  GO TO 2460
      DO 2450 J=JO,JN
      IF(KI(J).EQ.0)  GO TO 2450
      DATED(I)=DATE_
```

```
      IPASS=1
      GO TO 2460
 2450 CONTINUE
 2460 CONTINUE
      WRITE (7,9600) (P(J),J=JO,JN),PNAME(I)
      JO=JN+1
      JN=JN+7
      IF(IPASS.EQ.1)  GO TO 2480
      DO 2470 J=JO,JN
      IF(KI(J).EQ.0)  GO TO 2470
      DATED(I)=DATE_
      IPASS=1
      GO TO 2480
 2470 CONTINUE
 2480 CONTINUE
                    WRITE (7,9700)
(P(J),J=JO,JN),LAMBDA(I),ION(I),PNAME(I),DATED(I)
      GO TO 2600
 2500 CONTINUE
      JN=JO+NPARM-1
                    WRITE (7,9800)
(P(J),J=JO,JN),LAMBDA(I),ION(I),PNAME(I),DATED(I)
 2600 CONTINUE
 2650 CONTINUE
 2700 CONTINUE
      IF (IDO.EQ.2) GO TO 5100
      IDUMP=3
      IF (IICY.GE.1) GO TO 2800
C
-----------------------------------------------------------------
C     SET UP AND PRINT ERROR PLOTS.
C     READ IN AND STORE
C        NHL -- NUMBER OF HORIZONTAL DIVISIONS ON ORDINATE LESS 1.
C         NSBH -- NUMBER OF HORIZONTAL LINES PER DIVISION.
C         NVL -- NUMBER OF VERTICAL DIVISIONS ON ABSCISSA LESS 1.
C         NSBV -- NUMBER OF VERTICAL LINES PER DIVISION.
C         XMAX -- MAXIMUM TERPERATURE ON ABSCISSA.
C         XMIN -- MINIMUM TERPERATURE ON ABSCISSA.
C         YMAX -- MAXIMUM ERROR ON ORDINATE.
C            YMIN = - YMAX.
C
-----------------------------------------------------------------
      OPEN (UNIT=3,FILE=F03,
     1      ACCESS="SEQUENTIAL",
     2      FORM="FORMATTED",
     3      STATUS="UNKNOWN",POSITION="REWIND",
     4      ACTION="WRITE")
      OPEN (UNIT=10,FILE=F10,
     1      ACCESS="SEQUENTIAL",
     2      FORM="FORMATTED",
     3      STATUS="UNKNOWN",POSITION="REWIND",
     4      ACTION="WRITE")
      OPEN (UNIT=11,FILE=F11,
     1      ACCESS="SEQUENTIAL",
```

```
     2      FORM="FORMATTED",
     3      STATUS="UNKNOWN",POSITION="REWIND",
     4      ACTION="WRITE")
      OPEN (UNIT=12,FILE=F12,
     1      ACCESS="SEQUENTIAL",
     2      FORM="FORMATTED",
     3      STATUS="UNKNOWN",POSITION="REWIND",
     4      ACTION="WRITE")
      READ (50,5700) NHL,NSBH,NVL,NSBV
      READ (50,6400) XMAX,XMIN,YMAX
      YMIN=-YMAX
 2800 CONTINUE
      IF ((ISING.NE.0).AND.(IDO.NE.3)) GO TO 5300
      IN=0
C
----------------------------------------------------------------
C     CYCLE THROUGH EACH DATA SET.
C
----------------------------------------------------------------
      DO 4400 J=1,NSETS
      WRITE (3,7100)
      WRITE (3,6900) (TITLE(I),I=1,10),DATE
      IF ((((IGO(J)-1)/3).EQ.1).OR.(IGO(J).EQ.22))  GO TO 2900
      IGOES=IGO(J)
      IF(IGOES.GT.22)  IGOES=8
      WRITE (3,8400) TYPE(IGOES)
      GO TO 3000
 2900 CONTINUE
      IGOES=IGO(J)
      IF(IGOES.GT.22)  IGOES=8
      WRITE (3,8500) TYPE(IGOES)
 3000 CONTINUE
C
----------------------------------------------------------------
C     INITIALIZE THE PLOT IMAGE.
C
----------------------------------------------------------------
      CALL PLOT1(NSCALE,NHL,NSBH,NVL,NSBV)
      CALL PLOT2(IMAGE,XMAX,XMIN,YMAX,YMIN)
C
----------------------------------------------------------------
C     INITIALIZE CONSTANTS AND COUNTERS.
C
----------------------------------------------------------------
      IO=IN+1
      IN=IKOUNT(J)
      DO 3100 I=1,3
      SERR(I)=ZERO
      SERRSQ(I)=ZERO
 3100 CONTINUE
      SDELH=ZERO
      SDELHS=ZERO
      CALL PUTOUT(J)
C
```

```
------------------------------------------------------------------
C      CALCULATE AND PRINT YC.  CALCULATE AND SUM THE DIFFERENCE
(ERR),
C         PERCENT ERROR (RELERR), AND THE WEIGHTED DIFFERENCE (E).
C
------------------------------------------------------------------
      DO 4000 I=IO,IN
      CALL EAFW (YC,I,JSET)
      ERRDP=YO(I)-YC
      ERR=ERRDP
      IF (YO(I).EQ.ZERO) GO TO 3200
      RELERR=ERRDP*1.0D2/DABS(YO(I))
      GO TO 3300
 3200 CONTINUE
      RELERR=ZERO
 3300 CONTINUE
      E(1)=ERR/SIGYO(I)
      XI(1)=X(1,I)
      TO=X(2,I)
      IF ((((IGO(J)-1)/3).EQ.1).OR.(IGO(J).EQ.22))  GO TO 3400
                                            W     R     I     T     E
(3,8600)XI(1),TO,X(3,I),X(4,I),YO(I),YC,SIGYO(I),ERR,RELERR,
     1            E(1)
      GO TO 3900
C
------------------------------------------------------------------
C      CALCULATE THE ENTHALPY OF REACTION AT 298.15 K USING THE
GIBBS
C         ENERGY FUNCTION AND THE DATA FOR EACH OBSERVATION.
C
------------------------------------------------------------------
 3400 CONTINUE
      YY=YO(I)
      IF(IGO(J).EQ.22)  GO TO 3450
      IGOES=IGO(J)-3
      GEFN=-GEF(X(1,I),J)*X(1,I)
      GO TO (3500,3600,3700), IGOES
 3450 CONTINUE
      YY=YY+PTGEF(X(1,I),X(3,I),J)
      GEFN=-GEF(X(1,I),J)*X(1,I)
 3500 CONTINUE
      DELH=YY+GEFN
      GO TO 3800
 3600 CONTINUE
      DELH=GEFN-R*YY*X(1,I)
      GO TO 3800
 3700 CONTINUE
      DELH=GEFN-F*YY
 3800 CONTINUE
C
------------------------------------------------------------------
C      CORRECT THE ENTHALPY OF REACTION AT 298.15 K, AS CALCULATED
FROM
C         THE GIBBS ENERGY FUNCTION, FOR ANY HIGH TEMPERATURE
```

```
C        INVERSIONS.
C
-------------------------------------------------------------------
      CALL YDERIV(TREF,3)
      LPHASE=NPHASE(J)
      DH298=ZERO
      DO 3850 L=1,LPHASE
      IF(NINVER(L,J).EQ.0)  GO TO 3850
      IND298=INVPH(L,J,1)
      INDLST=INVPH(L,J,(NINVER(L,J)+1))
      DH=ZERO
      INDLO=(IND298-1)*NPARM
      INDHI=(INDLST-1)*NPARM
      DO 3810 K=1,NCPARM
      DH=DH+(AA(INDLO+K)-AA(INDHI+K))*DYDC(K)
 3810 CONTINUE
      DLYDL1=ZERO
      DLYDL2=ZERO
      DLYDH1=ZERO
      DLYDH2=ZERO
      IF(NOLAM(L,J))  GO TO 3840
      IF(.NOT.LAMBDA(IND298))  GO TO 3820
      JL=P(INDLO+NPARM-NLPARM+1)
      JH=P(INDLO+NPARM-NLPARM+2)
      JT=P(INDLO+NPARM-NLPARM+3)
      CALL LYDRIV(TREF,3,INDLO+1,JL,JH,JT)
      DLYDL1=DLYDC(1)
      DLYDL2=DLYDC(2)
 3820 CONTINUE
      IF(.NOT.LAMBDA(INDLST))  GO TO 3830
      JL=P(INDHI+NPARM-NLPARM+1)
      JH=P(INDHI+NPARM-NLPARM+2)
      JT=P(INDHI+NPARM-NLPARM+3)
      CALL LYDRIV(TREF,3,INDHI+1,JL,JH,JT)
      DLYDH1=DLYDC(1)
      DLYDH2=DLYDC(2)
 3830 CONTINUE
      DH=DH+AA(INDLO+NCPARM+3)*DLYDL1+AA(INDLO+NCPARM+4)*DLYDL2
     1     -AA(INDHI+NCPARM+3)*DLYDH1-AA(INDHI+NCPARM+4)*DLYDH2
      IF(.NOT.LAMBDA(IND298))  GO TO 3840
      IF(INSTAT(L,J).EQ.0)  GO TO 3840
      JL=P(INDLO+NPARM-NLPARM+1)
      JH=P(INDLO+NPARM-NLPARM+2)
      JT=P(INDLO+NPARM-NLPARM+3)
      CALL LYDRIV(TREF,3,INDLO+1,JL,JH,JT)
      DH=DH-DYDC(9)*DLHDC(1)*AA(INDLO+NCPARM+3)
     1     -DYDC(9)*DLHDC(2)*AA(INDLO+NCPARM+4)
      TINVER=TINV(L,J,1)
      JL=P(INDLO+NPARM-NLPARM+1)
      JH=P(INDLO+NPARM-NLPARM+2)
      JT=P(INDLO+NPARM-NLPARM+3)
      CALL LYDRIV(TINVER,3,INDLO+1,JL,JH,JT)
      DH=DH+DYDC(9)*DLHDC(1)*AA(INDLO+NCPARM+3)
     1     +DYDC(9)*DLHDC(2)*AA(INDLO+NCPARM+4)
```

```
 3840 CONTINUE
      DH298=DH298+COEF(L,J)*DH
 3850 CONTINUE
      DELH=DELH+DH298
      SDELH=SDELH+DELH
      SDELHS=SDELHS+DELH*DELH
                                                     WRITE
(3,8600)XI(1),TO,X(3,I),X(4,I),YO(I),YC,SIGYO(I),ERR,RELERR,
     1               E(1),DELH
      IF(ITEK(2).GT.0)  WRITE (10,10300)JSET,X(1,I),DELH
      DELH2=DELH
      IF(SIGYO(I).GT.1.D10)  DELH2=0.D0
              IF(ITEK(3).GT.0)                    WRITE
(11,10500)JSET,(X(K,I),K=1,6),DELH,DELH2
 3860 CONTINUE
 3900 CONTINUE
C
-----------------------------------------------------------------
C     ENTER THE POINT ON THE PLOT IMAGE.
C     SUM THE ERRORS.
C
-----------------------------------------------------------------
      CALL PLOT3(IMAGE,BCD,XI,E,1)
      SERR(1)=SERR(1)+ERR
      SERR(2)=SERR(2)+RELERR
      SERR(3)=SERR(3)+E(1)
      SERRSQ(1)=SERRSQ(1)+ERR*ERR
      SERRSQ(2)=SERRSQ(2)+RELERR*RELERR
      SERRSQ(3)=SERRSQ(3)+E(1)*E(1)
C
-----------------------------------------------------------------
C     CALCULATE AND WRITE THE STANDARD ERROR OF ESTIMATE FOR THE
C             DIFFERENCE,  THE  PERCENT  ERROR,  AND  THE  WEIGHTED
DIFFERENCE.
C    FOR CALCULATIONS OF THIRD-LAW ENTHALPY OF REACTION, CALCULATE
C        EACH ENTHALPY OF REACTION AT "TREF", AND EVALUATE
C        THE MEAN AND AVERAGE DEVIATION FOR EACH DATA SET.
C
-----------------------------------------------------------------
 4000 CONTINUE
      NDATA=1+(IN-IO)
      AN=NDATA
      DO 4100 I=1,3
      EBAR(I)=SERR(I)/AN
      IF(AN.EQ.1.)  GO TO 4050
      EBARSQ=EBAR(I)*EBAR(I)
      ANSESQ=SERRSQ(I)/AN
      IF(ANSESQ.LE.EBARSQ)  GO TO 4050
      STDEV(I)=SQRT(ANSESQ-EBARSQ)
      GO TO 4100
 4050 CONTINUE
      STDEV(I)=0.0
 4100 CONTINUE
      WRITE (3,7900)
```

```
      IF ((((IGO(J)-1)/3).EQ.1).OR.(IGO(J).EQ.28)) GO TO 4200
C*****      IF(IZGOES.NE.0)  GO TO 4200
      WRITE (3,8700) (EBAR(I),I=1,3),(STDEV(I),I=1,3),NDATA
      GO TO 4300
 4200 CONTINUE
      DN=DBLE(FLOAT(NDATA))
      DELHAV=SDELH/DN
      IF(DN.EQ.1.0D0)  GO TO 4210
      DHAVSQ=DELHAV*DELHAV
      ANSDHS=SDELHS/DN
      IF(ANSDHS.LE.DHAVSQ)  GO TO 4210
      DELHBA=DSQRT(ANSDHS-DHAVSQ)
      GO TO 4220
 4210 CONTINUE
      DELHBA=0.0D0
 4220 CONTINUE
                                        W     R     I     T     E
(3,8800)(EBAR(I),I=1,3),DELHAV,(STDEV(I),I=1,3),DELHBA,NDATA
      IF(ITEK(4).GT.0)  WRITE (12,8900) J,(REF(I,J),I=1,15)
      IF(ITEK(4).GT.0)  WRITE (12,10400)NDATA,DELHAV,DELHBA
 4300 CONTINUE
C
-----------------------------------------------------------------
C      CALL PUTOUT TO CALCULATE AND WRITE THE COMPLETE SET OF
CONSTANTS
C        FOR THE PHASES AND FOR THE DATA SET.  BYPASS THE LATTER
SET
C       OF CONSTANTS IF IGO(J) IS GREATER THAN OR EQUAL TO 7 OR IF
C        THE J-TH DATA SET HAS ONLY ONE PHASE.
C
-----------------------------------------------------------------
      CALL PUTIT(J)
C
-----------------------------------------------------------------
C     PRINT THE PLOT IMAGE FOR THE J-TH DATA SET.
C
-----------------------------------------------------------------
      WRITE (3,6500)
      WRITE (3,6900) (TITLE(I),I=1,10),DATE_
      WRITE (3,8900) J,(REF(I,J),I=1,15)
      CALL PLOT4(NL,LABEL,IMAGE)
      WRITE (3,9000)
 4400 CONTINUE
C
-----------------------------------------------------------------
C     PUT OUT TABLES FOR EACH SPECIES IN THE LIST PNAME(LISTP).
C          THIS OUTPUT WILL NOT HAVE THE CONTRIBUTIONS DUE TO THE
MAGNETIC
C        ANOMALIES.  IT IS TO BE USED WITH CARE.
C
-----------------------------------------------------------------
      OPEN (UNIT=4,FILE=F04,
     1     ACCESS="SEQUENTIAL",
     2     FORM="FORMATTED",
```

```
     3      STATUS="UNKNOWN",POSITION="REWIND",
     4      ACTION="WRITE")
      SC=1.0D0
      DO 5000 L=1,LISTP
C
------------------------------------------------------------------
C     WRITE LEGEND FOR EACH TABLE
C
------------------------------------------------------------------
      WRITE (4,6600) DATE_
      WRITE (4,6700) (TITLE(I),I=1,10)
      WRITE (4,9100) PNAME(L)
      WRITE (4,9200) (TYPE(I),I=1,7)
      INDEX=1+NPARM*(L-1)
      KOUNT=19
      IF (ION(L).EQ.-1) KOUNT=15
      M=(ION(L)+4)/2
      DO 4900 K=1,KOUNT
      T=TK(K,M)
      DO 4700 J=1,7
      VAL(J)=0.0D0
      IGOES=J
      IF (ION(L).EQ.-1) IGOES=IGOES+7
      IF (IGOES.EQ.14) GO TO 4700
      CALL YDERIV(TK(K,M),IGOES)
      DO 4500 I=1,NCPARM
      VAL(J)=VAL(J)+DYDC(I)*AA(INDEX+I-1)
 4500 CONTINUE
      IF (J.NE.7) GO TO 4700
      CALL YDERIV(TREF,J)
      DO 4600 I=1,NCPARM
      VAL(J)=VAL(J)-DYDC(I)*AA(INDEX+I-1)
 4600 CONTINUE
 4700 CONTINUE
      DO 4800 I=1,7
      AVAL(I)=VAL(I)
 4800 CONTINUE
      WRITE (4,9300) T,(AVAL(I),I=1,7)
 4900 CONTINUE
      JO=INDEX
      JN=JO+NPARM-1
      WRITE (4,7900)
      WRITE (4,9400) (AA(J),J=JO,JN)
      IF (IFMOUT.EQ.1)  GO TO 4950
      JNN=JO+5
      WRITE (7,9600) (AA(J),J=JO,JNN),PNAME(L)
      JO=JO+6
      JNN=JO+5
      WRITE (7,9600) (AA(J),J=JO,JNN),PNAME(L)
      JO=JO+6
      JNN=JO+5
      WRITE (7,9600) (AA(J),J=JO,JNN),PNAME(L)
      JO=JO+6
                         W R I T E       ( 7 , 9 7 1 0 )
```

```
(AA(J),J=JO,JN),LAMBDA(I),ION(I),PNAME(L),DATED(I)
      GO TO 5000
 4950 CONTINUE
                            W   R   I   T   E       (   7   ,   9   9   0   0   )
(AA(J),J=JO,JN),LAMBDA(I),ION(I),PNAME(L),DATED(I)
 5000 CONTINUE
      IF (IDO.EQ.3) GO TO 5300
C
-----------------------------------------------------------------
C     IF STEP-BACKWARD ELIMINATION OF NON-SIGNIFICANT PARAMETERS IS
C         IN EFFECT (ICY.NE.0), SET LEAST SIGNIFICANT PARAMETER TO
C         ZERO AND REPEAT REGRESSION.
C
-----------------------------------------------------------------
 5100 IF ((IREDO.EQ.0).OR.(IICY.EQ.ICY)) GO TO 5300
      KI(IREDO)=0
      P(IREDO)=0.0D0
      IICY=IICY+1
      GO TO 2300
 5200 CONTINUE
      WRITE (6,9500) J,ANAME
      WRITE (60,9500) J,ANAME
 5300 CONTINUE
 5400 CONTINUE
C
-----------------------------------------------------------------
C     RETRIEVE DATE-TIME FOR OUTPUT AT CLOSE OF EXECUTION.
C     CLOSE FILES AND STOP EXECUTION.
C
-----------------------------------------------------------------
      CALL TIMELY(DATE_)
      WRITE (60,10200)DATE_
C DG  DISP CHANGED TO STATUS
      CLOSE (UNIT=1,STATUS='KEEP')
      CLOSE (UNIT=2,STATUS='KEEP')
      CLOSE (UNIT=3,STATUS='KEEP')
      CLOSE (UNIT=4,STATUS='KEEP')
      CLOSE (UNIT=50,STATUS='KEEP')
      CLOSE (UNIT=60,STATUS='KEEP')
      CLOSE (UNIT=7,STATUS='KEEP')
      CLOSE (UNIT=9,STATUS='KEEP')
      CLOSE (UNIT=10,STATUS='KEEP')
      CLOSE (UNIT=11,STATUS='KEEP')
      CLOSE (UNIT=12,STATUS='KEEP')
      CLOSE (UNIT=66,STATUS='DELETE')
      STOP
C
-----------------------------------------------------------------
C     FORMAT STATEMENTS
C
-----------------------------------------------------------------
 5600 FORMAT (10A8)
 5602 FORMAT (A160)
 5610 FORMAT (10A8/10A8/5A8,L1,I2,37X,A8,A23)
```

```
 5700 FORMAT (16I5)
 5701 FORMAT (I5,2D10.3)
 5800 FORMAT (/16I5)
 5900 FORMAT (40I2)
 6000 FORMAT (A8,2X,D10.3,I5,A5,2I5)
 6100 FORMAT (6D12.5)
 6110 FORMAT (6D15.8/6D15.8/6D15.8/4D15.8,3D9.2,L1,I2,8X,A23)
 6200 FORMAT (I5,I3,9A8/(10A8))
 6300 FORMAT (80I1)
 6310 FORMAT (100I1)
 6400 FORMAT (8E10.3)
 6500 FORMAT (1H1)
 6600 FORMAT (42H1 THESE RESULTS WERE OBTAINED IN A RUN ON ,A23)
 6700 FORMAT (1H0,10A8/1H0)
 6800 FORMAT (60H0     PHASES CONSIDERED IN THIS REGRESSION ARE AS
FOLLO
     1WS---/1H0,10X,5A20/(1H ,10X,5A20))
 6900 FORMAT (1H ,10A8,25X,A23/1H0)
 7000 FORMAT (54H0THE FOLLOWING DATA SETS HAVE BEEN READ IN TO
STORAGE:/
     111H0SET NUMBER,10X,9HREFERENCE)
 7100 FORMAT (1H0)
 7200 FORMAT (1H ,A8)
 7300 FORMAT (1H ,I6,4X,15A8)
 7400 FORMAT (25H0THE NUMBER OF PHASES IS:,I5/31H THE NUMBER OF
OBSERVAT
     1IONS IS:,I5/21H THE TYPE OF DATA IS:,3X,A8/11H0PHASE
NAME,10X,11HC
     2OEFFICIENT,9X,10HREF. STATE,10X,10HINVERSIONS/1H )
 7500 FORMAT (1H ,1X,A8,11X,F8.3,15X,A3,14X,I6)
 7600 FORMAT (1H0,10X,26HINVERSIONS ARE AS FOLLOWS:/1H )
 7700 FORMAT (1H ,F15.2,3X,A8,5X,1H=,5X,A8,F20.3)
 7800 FORMAT (1H0,10X,A8,5X,58HIS A REFERENCE PHASE AND HAS ZERO
GIBBS E
     1NERGY AT 298.15 K/1H0)
 7900 FORMAT (1H )
   8000 FORMAT (1H
,15X,5HINDEX,21X,11HTEMPERATURE,18X,A8,13X,5HERROR/1H ,
     135X,2HT2,18X,2HT1/1H )
 8100 FORMAT (1H ,I20,F20.3,16X,1H-,3X,1P2D20.5)
 8200 FORMAT (1H ,I20,2F20.3,1P2D20.5)
 8400 FORMAT (1H ,T12,21HINDEPENDENT VARIABLES,
     1        T52,A8,
     1        T74,5HSIGYO,
     1        T99,5HERROR/1H ,
     2        T3,38H--------------------------------------,
     2        T43,26H--------------------------,
     2        T71,11H-----------,
     2        T84,32H--------------------------------/1H ,
     3        T4,6HX(1,I),T14,6HX(2,I),T24,6HX(3,I),T34,6HX(4,I),
     3        T45,8HOBSERVED,T58,10HCALCULATED,
     3        T72,9H(WT)**-.5,
     3        T89,3HO-C,T97,8H%(O-C)/O,T107,9H(O-C)/SIG)
 8500 FORMAT (1H ,T12,21HINDEPENDENT VARIABLES,
```

```
     1         T52,A8,
     1         T74,5HSIGYO,
     1         T99,5HERROR,
     1         T119,12HDELTA H(298)/1H ,
     2         T3,38H--------------------------------------,
     2         T43,26H--------------------------,
     2         T71,11H-----------,
     2         T84,32H--------------------------------,
     2         T118,14H--------------/1H ,
     3         T4,6HX(1,I),T14,6HX(2,I),T24,6HX(3,I),T34,6HX(4,I),
     3         T45,8HOBSERVED,T58,10HCALCULATED,
     3         T72,9H(WT)**-.5,
     3         T89,3HO-C,T97,8H%(O-C)/O,T107,9H(O-C)/SIG)
   8   6   0   0          F   O   R   M   A   T          (   1   H
,F9.2,3F10.2,1P2D14.5,D13.4,0PF12.4,2F11.4,1PD16.6)
 8700 FORMAT (58H0THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET
ARE ---
     1---,T83,3F11.4/59H0THE STANDARD ERRORS OF ESTIMATE ABOUT THE
MEAN
     2ARE--------,T83,3F11.4/31H0THE NUMBER OF OBSERVATIONS IS ,I5)
 8800 FORMAT (58H0THE ARITHMETIC MEAN OF THE ERRORS FOR THIS SET
ARE ---
     1---,T83,3F11.4,1PD16.6/59H0THE STANDARD ERRORS OF ESTIMATE
ABOUT T
     2HE MEAN ARE--------,T83,0P3F11.4,1PD16.6/31H0THE NUMBER OF
OBSERVA
     3TIONS IS ,I5)
 8900 FORMAT (1H0,I5,3X,15A8/1H )
 9000 FORMAT (1H0,T35,21HTEMPERATURE (KELVINS))
 9100 FORMAT (1H0,A8)
 9200 FORMAT (1H ,15X,A8,8X,A8,8X,A8,8X,A8,8X,A8,8X,A8,8X,A8/1H )
 9300 FORMAT (1H ,F7.2,2F16.3,2F16.0,2F16.4,F16.0)
      9    4    0    0              F     O     R     M     A     T
(1H0,10X,3H'A',15X,3H'B',15X,3H'C',15X,3H'D',15X,3H'E',15X,
     13H'F',15X,3H'G'/1H0,1P7D18.7/1H0,1P7D18.7/1H0,1P7D18.7)
 9500 FORMAT (39H I,YOUR FRIENDLY COMPUTER, DO NOW QUIT./9H0IN YOUR
,I4,
     146HTH DATA SET YOU HAVE MISSTYPED THE PHASE NAME ,A8)
 9600 FORMAT (1P6D15.8,A8)
 9700 FORMAT (1P4D15.8,1P3D9.2,L1,I2,A8,A23)
 9710 FORMAT (1P4D15.8,1P3D9.2,L1,I2,A8,A23,8HCOMPLETE)
 9800 FORMAT (10A8/10A8/5A8,L1,I2,37X,A8,A23)
 9900 FORMAT (10A8/10A8/5A8,L1,I2,37X,A8,A23,8HCOMPLETE)
10000 FORMAT (5I5,2A8,1X,4I1)
10100 FORMAT (16(L1,6X))
10200 FORMAT (42H0THESE RESULTS WERE COMPLETED IN A RUN AT ,A23)
10300 FORMAT (I5,1H;,F10.4,1H,,F12.0)
10400 FORMAT (6x,I8,F12.0,F12.0)
10500 FORMAT (I6,1H;,1PD13.6,5(1H,,1PD13.6))
10600 FORMAT (' THE DATA FILE HAS BEEN READ AT ^G^G^G',A23)
10700 FORMAT (' THE DATA FILE HAS BEEN FITTED AT ^G^G^G',A23)
      END
      BLOCKDATA
      IMPLICIT REAL*8(A-H,O-Z)
```

```
      CHARACTER*1 BCD,LABEL
      CHARACTER*8 PNAME,TITLE,REF,RECKON,UNITS,YESNO,TYPE,ASTAR
C
-----------------------------------------------------------------------
C
C       PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C         DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C        MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------------
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION PNAME(IP1),TITLE(10),REF(20,IP3),UNITS(4),YESNO(2),
     1          TYPE(IP9),LABEL(50)
                  COMMON /WATER/
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,AV,SCINV,TREF,PREF,
     1             STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /OCEAN/ RJ,RC,FJ,FC
      COMMON /HOTAIR/ PNAME,TITLE,REF,UNITS,RECKON,YESNO,ASTAR,
     1              TYPE,LABEL,BCD
      DATA UNITS/'joules  ','JOULES  ','calories','CALORIES'/
C
-----------------------------------------------------------------------
C         1986 RECOMMENDED VALUES OF THE FUNDAMENTAL PHYSICAL
CONSTANTS.
C
C        F = FARADAY
C        R = (MOLAR GAS CONSTANT)*(ln(10.0))
C        AV = AVOGADRO CONSTANT
C
-----------------------------------------------------------------------
      DATA FJ,FC/9.6485309D4,2.30605423D4/
      DATA RJ,RC/19.14486678D0,4.575732978D0/
      DATA AV/6.0221367D-1/
                                                DATA
ZERO,ONE,TWO,THREE,FOUR,SIX/0.0D0,1.0D0,2.0D0,3.0D0,4.0D0,
     1  6.0D0/
      DATA SCINV/-1.0D0,1.0D0/
      DATA TREF,PREF/2.9815D2,1.0D0/
                   DATA                    STCOEF
/1.0D0,2.0D0,3.0D0,4.0D0,5.0D0,0.5D0,0.4D0,0.33333333
     133D0,0.25D0,0.2D0/
      DATADIEO,ADIE,BDIE,THETA/3.057D2,1.875D-2,-1.2741D1,2.19D2/
      DATA YESNO    /'NO ','YES'/
      DATA TYPE     /'   CP   ','ENTROPY ','ENTHALPY','GIBBS EN',
     1    ' LOG K  ','CELL EMF','HT2-HT1 ','   GEF  ','   CV   ',
     1    'T(CRIT) ','  V(M)  ','V(CELL) ','  V-VO  ','  V/VO  ',
```

```
     1    ' ALPHA ','DV/VO@P ','DV/(VDT)','KAPPA-T ',' BM-T  ',
     1    'DV/VO@T ','DV/(VDT)',' G(T,P) ','KAPPA-S ',' BM-S  ',
     1    'GRUN GAM','dP/dT@PO','SPECIAL ','SPECIAL '/
      DATA ASTAR/'********'/
                                   D  A  T  A              T  K
/273.15D0,298.15D0,323.15D0,348.15D0,373.15D0,398.15D0,
                                                                 1
423.15D0,448.15D0,473.15D0,498.15D0,523.15D0,548.15D0,573.15D0,
     2 598.15D0,623.15D0,0.0D0,0.0D0,0.0D0,0.0D0,273.15D0,298.15D0,
     3 4.0D2,5.0D2,6.0D2,7.0D2,8.0D2,9.0D2,1.0D3,1.1D3,1.2D3,1.3D3,
     4 1.4D3,1.5D3,1.6D3,1.7D3,1.8D3,1.9D3,2.0D3/
       DATA    LABEL    /'O','B','S','    ','L','E','S','S','
','C','A','L','C',
         C          '    ' , ' O ' , ' V ' , ' E ' , ' R ' , '
','U','N','C','E','R','T','A','I','N',
     C   'T','Y',' ',' ',' ',' ',' ',' ',' ',' ',' ',' ',' ',' ','
',
     C   ' ',' ',' ',' ',' ',' ',' '/
      DATA NL/30/
      DATA BCD/'O'/
      DATA NSCALE/5*0/
      END
      SUBROUTINE ORGLS
C
-----------------------------------------------------------------
C
C                             OR GLS
C
C           A GENERAL FORTRAN LEAST SQUARES PROGRAM
C                               BY
C             WILLIAM R. BUSING AND HENRI A. LEVY
C                        CHEMISTRY DIVISION
C                   OAK RIDGE NATIONAL LABORATORY
C                       OAK RIDGE, TENNESSEE
C
C     REFERENCE-- BUSING, W. R. AND LEVY, H. A., 1962, OR GLS, A
GENERAL
C                     FORTRAN LEAST SQUARES PROGRAM, OAK RIDGE
C                     NATIONAL LABORATORY, OAK RIDGE, TENN.,
C                     ORNL-TM-271.
C
C
C                             ORGLS
C
C          ORGLS HAS BEEN ADAPTED FROM BUSING AND LEVY'S OR GLS
C      PROGRAM TO ALLOW USE OF THE STATISTICAL ROUTINES WITHOUT
BEING
C     RESTRICTED TO THE RIGID INPUT-OUTPUT FEATURES OF THE PROGRAM.
C     THE CONVERSION HAS PERMITTED CHANGES WHICH CLARIFY THE OUTPUT
C      FOR THIS PECULIAR PROBLEM.
C
C      ADAPTATION BY HAAS, 8/20/72.
C
C      WEIGHT NORMALIZATION BY FISHER 4/11/74
```

```
C
-------------------------------------------------------------------
      IMPLICIT REAL*8 (A-H,O-Z)
      CHARACTER*23 DATE_
      LOGICAL*1 LAMBDA,NOLAM,UNDAMP
      CHARACTER*1 BCD,LABEL
      CHARACTER*8 TRUE
      CHARACTER*8 PNAME,TITLE,REF,RECKON,UNITS,YESNO,TYPE,ASTAR
      CHARACTER*23 DATE2
      REAL*4 PCTERR,OUT
C
-------------------------------------------------------------------
C
C     PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C      IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C       DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C       MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C       ALSO.
C
      INCLUDE PARAM.FOR
C
C
-------------------------------------------------------------------
      DIMENSION OUT(9),TRUE(2),DAMP(9)
      DIMENSION SQSIG(2),V(IP6),DV(IP6),DIAG(IP6),
     1          ROW(IP6)
      DIMENSION COEF(IP4,IP3),TINV(IP4,IP3,IP10),NPHASE(IP3),
         1
IKOUNT(IP3),IGO(IP3),ISTATE(IP4,IP3),INSTAT(IP4,IP3),
     2         INVPH(IP4,IP3,IP11),INVSC(IP4,IP3),ISPECL(IP4,IP3),
     3          IPHASE(IP4,IP3),NINVER(IP4,IP3)
                               DIMENSION
X(NX,IP2),P(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1          ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION ERRP(IP6),IHOLD(IP1),ITEK(4)
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION AA(IP6)
      DIMENSION LAMBDA(IP1),NOLAM(IP4,IP3)
      DIMENSION AM(IP8)
      DIMENSION PNAME(IP1),TITLE(10),REF(20,IP3),UNITS(4),YESNO(2),
     1          TYPE(IP9),LABEL(50)
      COMMON /EARTH/ COEF,TINV,NPHASE,IKOUNT,IGO,ISTATE,INSTAT,
     1              INVPH,INVSC,ISPECL,IPHASE,NINVER,NSETS,LISTP
      COMMON /AIR/ X,P,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1             ISING,ISTOP,IL,JDF,ION
                   COMMON        /FIRE/
ERRP,IWRITE,ICY,IICY,IREDO,IREG,NHOLD,IHOLD,ITEK,
     1             IDUMP
                  COMMON         /WATER/
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1              STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
```

```
      COMMON /TIME_/ DATE_
      COMMON /MAN/ AA
      COMMON /AETHER/ LAMBDA,NOLAM,UNDAMP
      COMMON /LAND/ AM
      COMMON /HOTAIR/ PNAME,TITLE,REF,UNITS,RECKON,YESNO,ASTAR,
     1                TYPE,LABEL,BCD
      DATA TRUE/'reckon  ','RECKON  '/
      DATA UNDER/300.0D0/
      DATA DAMP/1.D0,0.63D0,0.40D0,0.25D0,0.16D0,0.10D0,
     1          0.063D0,0.040D0,0.025D0/
C     FORMAT STATEMENTS
  100 FORMAT (1H1,10A8)
  150 FORMAT (42H0 THESE RESULTS WERE OBTAINED IN A RUN AT ,A23)
  200 FORMAT (32H0NUMBER OF CYCLES IN THIS JOB ISI3/37H0NUMBER OF
PARAME
     1TERS TO BE VARIED ISI4/51H0NUMBER OF INDEPENDENT VARIABLES
PER OBS
     2ERVATION ISI3)
  300 FORMAT (45H0DERIVATIVES PROGRAMMED IN SUBROUTINE  EAFW. )
  400 FORMAT (31H0WEIGHTS TO BE SUPPLIED BY USER)
  500 FORMAT (34H0UNIT WEIGHTS TO BE SET BY PROGRAM)
  600 FORMAT (29H0NUMBER OF PARAMETERS READ ISI5)
  700 FORMAT (31H0NUMBER OF OBSERVATIONS READ ISI6)
  800 FORMAT (46H0CALCULATED Y BASED ON PARAMETERS BEFORE CYCLEI3)
          900 FORMAT
(1H0,5HINDEX,4X,6HX(1,I),4X,6HX(2,I),4X,6HX(3,I),4X,6HX(4,I

1)9X,6HY(OBS),9X,7HY(CALC),8X,8HOBS-CALC,9X,6HSIG(O),6X,12H(O-C)/SI
     1G(O))
 1000 FORMAT (1H ,I5,F10.2,8X,F12.2,F10.2,1P4D16.3,0PF16.4)
 1100 FORMAT (1H ,I5,F10.2,F8.2,F12.2,F10.2,1P4D16.3,0PF16.4)
 1200 FORMAT (1H ,I5,F10.2,8X,F12.2,F10.2,5F16.4)
 1300 FORMAT (1H ,I5,F10.2,F8.2,F12.2,F10.2,5F16.4)
 1350 FORMAT (1H ,I5,F10.2,F8.2,F12.5,F10.5,5F16.4)
 1010 FORMAT (1H ,I5,F10.2,8X,F12.2,F10.2,1P3D16.3,2(11X,5H---- ))
 1110 FORMAT (1H ,I5,F10.2,F8.2,F12.2,F10.2,1P3D16.3,2(11X,5H----
))
 1210 FORMAT (1H ,I5,F10.2,8X,F12.2,F10.2,3F16.4,2(11X,5H---- ))
 1310 FORMAT (1H ,I5,F10.2,F8.2,F12.2,F10.2,3F16.4,2(11X,5H---- ))
 1360 FORMAT (1H ,I5,F10.2,F8.2,F12.5,F10.5,3F16.4,2(11X,5H---- ))
 1400 FORMAT (51H0AGREEMENT FACTORS BASED ON PARAMETERS BEFORE
CYCLEI3/2
            10H0SUM(W*(O-C)**2)  IS
1PD16.8/35H0SQRTF(SUM(W*(O-C)**2)/(NO-NV)) I
     2S 1PD16.8)
 1500 FORMAT (60H0ESTIMATED AGREEMENT FACTORS BASED ON PARAMETERS
AFTER }
          1CYCLEI3/20H0SUM(W*(O-C)**2)  IS
1PD16.8/35H0SQRTF(SUM(W*(O-C)**2)/(
     2NO-NV)) IS 1PD16.8)
 1600 FORMAT (62H MATRIX HAS A ZERO DIAGONAL ELEMENT CORRESPONDING
TO PA
     1RAMETERI3,16H OF THOSE VARIED)
 1700 FORMAT (40H SINGULARITY RETURN FROM MATRIX INVERTER)
```

```
 1800   FORMAT   (37H0PARAMETERS   AFTER   LEAST   SQUARES
CYCLEI3/1H0,T16,'OLD',T
       135,'CHANGE',T57,'NEW',T77,'ERROR',T95,'PCT.
CHANGE',T118,'PCT. ERR
     2OR'/1H )
 1900 FORMAT (1H0,A8,':  CONSTRAINTS (ELEM = 1, OTHER = 0) = ',I2,
     1     ' AND LAMBDA ANOMALY = ',L1,', Ja = ',I2,' and Jb =
',I2,'.')
 2000 FORMAT (1H I3,4X,1PD17.10)
 2100 FORMAT (1H ,I3,1P5D21.10,0PF17.4)
 2200 FORMAT (66H0SUBROUTINE TEST INDICATES THAT JOB IS TO BE
TERMINATED
     1 FOR REASONI2)
   2300   FORMAT   (16H0TRIAL
CONSTANTS/1H0,2X,1HI,9X,4HP(I),6X,5HKI(I)/1H )
 2400 FORMAT (1H0,9X,A8)
 2500 FORMAT (1H ,I3,5X,1PD15.8,6X,I1)
 2600 FORMAT (19H0CORRELATION MATRIX)
 2700 FORMAT (1H0I3,10D12.4/(1H 3X,10D12.4))
 2800  FORMAT  (14H1***WARNING***/93H0THE  TERM  SIG/(NO-NV)  IS
NEGATIVE.  T
     1HE ABSOLUTE VALUE IS TAKEN AND THE REGRESSION CONTINUES.)
      DO 2900 I=1,NP
      ERRP(I)=0.0D0
 2900 CONTINUE
      WRITE (60,100) (TITLE(I),I=1,10)
      WRITE (60,150) DATE_
      WRITE (60,200) NC,NV,NX
      WRITE (60,300)
      IF (IW) 3100,3000,3100
 3000 WRITE (60,400)
      GO TO 3200
 3100 WRITE (60,500)
 3200 CONTINUE
      WRITE (60,600) NP
      WRITE (60,700) NO
      IF (NC) 3300,3300,3500
 3300 DO 3400 I=1,NP
 3400 KI(I)=0
C     INITIALIZE PROBLEM AND ENTER SUBROUTINE  PRELIM IF PROVIDED
 3500 NM=(NV*(NV+1))/2
      SQSIG(1)=0.0D0
      CALL PRELIM
C     PUT OUT TRIAL PARAMETERS, AND KEY-INTEGERS.
      WRITE (60,2300)
      JO=1
      DO 3600 I=1,LISTP
      WRITE (60,2400) PNAME(I)
      JN=JO+NPARM-1
      WRITE (60,2500) (J,P(J),KI(J),J=JO,JN)
      JO=JO+NPARM
 3600 CONTINUE
C     START LOOP TO PERFORM NC CYCLES AND ONE FINAL CALCULATION OF
Y
```

```
      NCY=NC+1
      DO 7900 IC=1,NCY
      ICM1=IC-1
      CALL TIMELY(DATE2)
      WRITE (6,3610)ICM1,DATE2
 3610 FORMAT(' BEGINNING CYCLE ',I2,' OF THE CALCULATIONS AT
^G^G',A23)
      IF(IC.EQ.NCY)  JDF=1
      IF(IC.LE.9)  CALL ADJUST
C        CLEAR ARRAYS AM AND V EXCEPT ON LAST CYCLE
      IF (IC-NCY) 3700,4000,4000
 3700 DO 3800 I=1,NM
 3800 AM(I)=0.0D0
      DO 3900 I=1,NV
 3900 V(I)=0.0D0
C         INITIALIZE FOR CYCLE IC AND PUT OUT CAPTION FOR LIST OF
Y(CALC)
 4000 SQSIG(2)=SQSIG(1)
      SIG=0.0D0
      WRITE (60,100) (TITLE(I),I=1,10)
      IF (IL.NE.0) GO TO 4100
      IF (IC.NE.NCY) GO TO 4200
 4100 CONTINUE
      WRITE (60,800) IC
      WRITE (60,900)
 4200 CONTINUE
C        START LOOP THROUGH NO OBSERVATIONS
      IF (IW.EQ.0) SQRTNO=DSQRT(DBLE(FLOAT(NO)))
      IDUMP=60
      IF((IL.EQ.0).AND.(IC.NE.NCY))  IDUMP=66
      DO 5900 I=1,NO
C               ENTER USERS SUBROUTINE TO COMPUTE Y(CALC) AND
DERIVATIVES
      CALL EAFW(YC,I,JSET)
C                OBTAIN WEIGHT AND CALCULATE QUANTITIES FROM
Y(OBS)-Y(CALC)
      IF (IW) 4400,4300,4400
 4300 SQRTW=1.0D0/SIGYON(I)
      GO TO 4500
 4400 SIGYO(I)=1.0D0
      SIGYON(I)=SQRTNO
      SQRTW=1.0D0/SQRTNO
 4500 DY=YO(I)-YC
      WDY=SQRTW*DY
      SIG=SIG+WDY*WDY
C               PUT OUT Y(CALC) AND OTHER INFORMATION FOR ONE
OBSERVATION
      IF (IL.NE.0) GO TO 4600
      IF (IC.NE.NCY) GO TO 5100
 4600 CONTINUE
      OUT(1)=X(1,I)
      OUT(2)=X(2,I)
      OUT(3)=X(3,I)
      OUT(4)=X(4,I)
```

```
      OUT(5)=YO(I)
      OUT(6)=YC
      OUT(7)=DY
      OUT(8)=SIGYO(I)
      OUT(9)=DY/SIGYO(I)
      IF(ITEK(1).GT.0) WRITE (9,9100) JSET,(X(K,I),K=1,6),YO(I),YC
      IF(SIGYO(I).GE.1.0D10)  GO TO 4910
      IF(IGO(JSET).GT.28)  GO TO 4650
      IF (X(2,I).EQ.0.0D0) GO TO 4800
      IF ((DABS(YO(I)).LT.1.0D-2).AND.(YO(I).NE.0.0D0)) GO TO 4700
      IF ((DABS(YC).LT.1.0D-2).AND.(YC.NE.0.0D0))  GO TO 4700
      WRITE (60,1300) I,(OUT(K),K=1,9)
      GO TO 5000
 4650 CONTINUE
      WRITE (60,1350)I,(OUT(K),K=1,9)
      GO TO 5000
 4700 CONTINUE
      WRITE (60,1100) I,(OUT(K),K=1,4),YO(I),YC,DY,SIGYO(I),OUT(9)
      GO TO 5000
 4800 CONTINUE
      IF ((DABS(YO(I)).LT.1.0D-2).AND.(YO(I).NE.0.0D0)) GO TO 4900
      WRITE (60,1200) I,OUT(1),(OUT(K),K=3,9)
      GO TO 5000
 4900 CONTINUE
                   WRITE (60,1000)
I,OUT(1),OUT(3),OUT(4),YO(I),YC,DY,SIGYO(I),OUT(9)
      GO TO 5000
 4910 CONTINUE
      IF(IGO(JSET).GT.28)  GO TO 4920
      IF (X(2,I).EQ.0.0D0) GO TO 4940
      IF ((DABS(YO(I)).LT.1.0D-2).AND.(YO(I).NE.0.0D0)) GO TO 4930
      IF ((DABS(YC).LT.1.0D-2).AND.(YC.NE.0.0D0))  GO TO 4930
      WRITE (60,1310) I,(OUT(K),K=1,7)
      GO TO 5000
 4920 CONTINUE
      WRITE (60,1360)I,(OUT(K),K=1,7)
      GO TO 5000
 4930 CONTINUE
      WRITE (60,1110) I,(OUT(K),K=1,4),YO(I),YC,DY
      GO TO 5000
 4940 CONTINUE
      IF ((DABS(YO(I)).LT.1.0D-2).AND.(YO(I).NE.0.0D0)) GO TO 4950
      WRITE (60,1210) I,OUT(1),(OUT(K),K=3,7)
      GO TO 5000
 4950 CONTINUE
      WRITE (60,1010) I,OUT(1),OUT(3),OUT(4),YO(I),YC,DY
 5000 CONTINUE
 5100 CONTINUE
C           BY-PASS DERIVATIVE AND MATRIX SET-UP ON FINAL CALC OF
Y
      IF (IC-NCY) 5200,5900,5900
C              START LOOP TO STORE AN ARRAY OF NV DERIVATIVES
 5200 J=1
      DO 5400 K=1,NP
```

```
      IF (KI(K)) 5400,5400,5300
 5300 CONTINUE
C                      OBTAIN DERIVATIVE FROM THOSE PROGRAMMED BY
USER
      DV(J)=SQRTW*DC(K)
      J=J+1
 5400 CONTINUE
C             THE END OF LOOP TO OBTAIN DERIVATIVES
C              START LOOP TO STORE MATRIX AND VECTOR.
C             1604 OR GLS STORAGE SCHEME IS REVERSE OF 7090 OR GLS
      JK=1
      DO 5800 J=1,NV
      TEMP=DV(J)
      IF (TEMP) 5600,5500,5600
C                    BY-PASS IF DERIVATIVE IS ZERO
 5500 JK=JK+NV+1-J
      GO TO 5800
 5600 DO 5700 K=J,NV
      IF((TEMP.EQ.ZERO).OR.(DV(K).EQ.ZERO))  GO TO 5650
      IF(DABS(DLOG10(DABS(TEMP))+DLOG10(DABS(DV(K)))).GT.UNDER)
     1      GO TO 5650
      AM(JK)=AM(JK)+TEMP*DV(K)
 5650 CONTINUE
      JK=JK+1
 5700 CONTINUE
      V(J)=V(J)+TEMP*WDY
 5800 CONTINUE
C                THE END OF LOOP TO STORE MATRIX AND VECTOR
 5900 CONTINUE
C          THE END OF LOOP THROUGH NO OBSERVATIONS
C        COMPUTE AND PUT OUT AGREEMENT FACTORS
      ONVN=NO-NV
      SQSIG(1)=DSQRT(SIG/(ONVN))
      WRITE (60,1400) IC,SIG,SQSIG(1)
C         BY-PASS MATRIX INVERSION AND PARAMETER OUTPUT ON FINAL
CYCLE
      IF (IC-NCY) 6000,8000,8000
C           START LOOP TO TEST FOR ZERO DIAGONAL ELEMENT
 6000 ISING=0
      II=1
      IID=NV
      DO 6300 I=1,NV
      IF (AM(II)) 6200,6100,6200
 6100 ISING=1
      WRITE (60,1600) I
 6200 II=II+IID
      IID=IID-1
 6300 CONTINUE
C          THE END OF LOOP TO TEST FOR ZERO DIAGONAL ELEMENT
C           TERMINATE JOB IF ZERO DIAGONAL ELEMENT WAS FOUND
      IF (ISING) 8600,6400,8600
C              ENTER SUBROUTINE TO REPLACE MATRIX WITH INVERSE
 6400 CALL MINV(NV,ISING)
      IF (ISING) 6500,6600,6500
```

```
C                    TERMINATE JOB IF SINGULAR MATRIX WAS FOUND
 6500 WRITE (60,1700)
      GO TO 8600
C                    START LOOP FOR MATRIX VECTOR MULTIPLICATION FOR
C                                                  PARAMETER CHANGES
 6600 DO 7100 I=1,NV
      PDI=0.0D0
      IJ=I
      IJD=NV-1
      DO 7000 J=1,NV
      PDI=PDI+AM(IJ)*V(J)
      IF (J-I) 6700,6800,6900
 6700 IJ=IJ+IJD
      IJD=IJD-1
      GO TO 7000
C                           SAVE DIAGONAL ELEMENTS OF INVERSE MATRIX
 6800 DIAG(I)=AM(IJ)
 6900 IJ=IJ+1
 7000 CONTINUE
      PD(I)=PDI
      SIG=SIG-PDI*V(I)
 7100 CONTINUE
C                   THE END OF LOOP FOR MATRIX VECTOR MULTIPLICATION
C                    RECOMPUTE AGREEMENT FACTOR USING MODIFIED SIG
      IF (SIG) 7200,7300,7300
 7200 CONTINUE
      WRITE (60,2800)
      SIG=DABS(SIG)
 7300 CONTINUE
      SQSIG(1)=DSQRT(SIG/(NO-NV))
C                   PUT OUT CAPTION FOR LIST OF CORRECTED PARAMETERS
      WRITE (60,100) (TITLE(I),I=1,10)
      WRITE (60,1800) IC
C                    START LOOP TO CORRECT AND PUT OUT PARAMETERS
      J=1
      JO=1
      DO 7700 IO=1,LISTP
      JL=P((IO-1)*NPARM+23)
      JH=P((IO-1)*NPARM+24)
      WRITE (60,1900) PNAME(IO),ION(IO),LAMBDA(IO),JL,JH
      JN=JO+NPARM-1
      DO 7600 I=JO,JN
      IF (KI(I)) 7400,7400,7500
 7400 WRITE (60,2000) I,P(I)
      IF((RECKON.EQ.TRUE(1)).OR.(RECKON.EQ.TRUE(2)))
     1       WRITE (2,8700) I,P(I),ZERO
      GO TO 7600
 7500 POLD=P(I)
      KII=KI(I)
      P(I)=POLD+PD(J)*DAMP(KII)
      SIGP=DSQRT(DIAG(J))*SQSIG(1)
      PCTCHG=1.D2*PD(J)*DAMP(KII)/P(I)
      PCTERR=DABS(1.0D2*SIGP/P(I))
      ERRP(I)=PCTERR
```

```
      IF((RECKON.EQ.TRUE(1)).OR.(RECKON.EQ.TRUE(2)))
     1       WRITE (2,8700) I,P(I),SIGP
      WRITE (60,2100) I,POLD,PD(J),P(I),SIGP,PCTCHG,PCTERR
      J=J+1
 7600 CONTINUE
      JO=JO+NPARM
 7700 CONTINUE
C                THE END OF LOOP TO CORRECT AND PUT OUT PARAMETERS
C                  PUT OUT ESTIMATED AGREEMENT FACTORS
      WRITE (60,1500) IC,SIG,SQSIG(1)
C                        ENTER USERS SUBROUTINE TO TEST AND MODIFY
PARAMETERS
C                                                                OR END
JOB
      ISTOP=0
      CALL TEST
C                   TERMINATE JOB IF INDICATED BY USERS SUBROUTINE
TEST
      IF (ISTOP) 7800,7900,7800
 7800 WRITE (60,2200) ISTOP
      GO TO 8000
 7900 CONTINUE
C                 THE END OF LOOP THROUGH NC CYCLES AND FINAL CALC
OF Y
C     TERMINATE JOB
 8000 IF (NC) 8600,8600,8100
 8100 CONTINUE
      IF((IL.EQ.2).AND.(.NOT.((RECKON.EQ.TRUE(1))
     1     .OR.(RECKON.EQ.TRUE(2)))))
     1     GO TO 8600
C        CALCULATE AND PUT OUT CORRELATION MATRIX
      IF(IL.EQ.2)  WRITE (60,100) (TITLE(I),I=1,10)
      IF(IL.EQ.2)  WRITE (60,2600)
      DO 8200 I=1,NV
      DIAG(I)=1.0D0/DSQRT(DIAG(I))
 8200 CONTINUE
      IJ=1
      DO 8500 I=1,NV
      DO 8300 J=1,NV
      ROW(J)=0.0D0
 8300 CONTINUE
      DO 8400 J=I,NV
      ROW(J)=AM(IJ)*DIAG(I)*DIAG(J)
      IJ=IJ+1
 8400 CONTINUE
      IF(IL.EQ.2)  WRITE (60,2700) I,(ROW(J),J=1,NV)
      IF((RECKON.EQ.TRUE(1)).OR.(RECKON.EQ.TRUE(2)))
     1       WRITE (2,8700) I,(ROW(J),J=1,NV)
 8500 CONTINUE
 8600 CONTINUE
      RETURN
 8700 FORMAT (I3,2X,1p5d15.8/(5X,1p5d15.8))
 8800 FORMAT (20A4)
 8900 FORMAT (16I5)
```

```
 9000 FORMAT (10A8)
 9100 FORMAT (I5,1H;,1PD12.5,5(1H,,1PD12.5))
      END
      SUBROUTINE PRELIM
C
-----------------------------------------------------------------
C     DUMMY SUBROUTINE PRELIM
C
-----------------------------------------------------------------
      RETURN
      END
      SUBROUTINE ADJUST
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL*1 LAMBDA,NOLAM,UNDAMP
C
-----------------------------------------------------------------
C
C       PARAMETERS  STATEMENTS.   THESE  HAVE  BEEN  ENTERED  IN  EACH
ROUTINE
C         IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL

C         DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C         MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C         ALSO.
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------
                            D    I    M    E    N    S    I    O    N
X(NX,IP2),P(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1          ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION LAMBDA(IP1),NOLAM(IP4,IP3)
      COMMON /AIR/ X,P,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1              ISING,ISTOP,IL,JDF,ION
      COMMON /AETHER/ LAMBDA,NOLAM,UNDAMP
      IF(IC.EQ.1)  GO TO 9999
      IF(.NOT.UNDAMP)  GO TO 9999
      DO 1000 I=1,NP
      IF(KI(I).LE.1)  GO TO 1000
      KI(I)=KI(I)-1
 1000 CONTINUE
 9999 CONTINUE
      RETURN
      END
      SUBROUTINE TEST
C
-----------------------------------------------------------------
C
C                               TEST
C
C     TEST  TERMINATES THE REGRESSION IF THE CHANGE IN ALL
```

```
C           PARAMETERS IS LESS THAN 1.0D-8.
C
C      TEST   WILL ALSO CAUSE IREDO TO TAKE THE INDEX OF THE
C          PARAMETER WHICH HAS THE GREATEST ERROR, PROVIDED ICY HAS

C          AN NON-ZERO VALUE AND PROVIDED THE ERROR ON ONE OR MORE
C           PARAMETERS IS GREATER THAN 10 PERCENT.
C
C
-----------------------------------------------------------------------
      IMPLICIT REAL*8 (A-H,O-Z)
C
-----------------------------------------------------------------------
C
C       PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C         IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL

C         DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C         MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C         ALSO.
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------------
                           DIMENSION
X(NX,IP2),P(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1      ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION ERRP(IP6),IHOLD(IP1),ITEK(4)
      COMMON /AIR/ X,P,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1             ISING,ISTOP,IL,JDF,ION
                             COMMON     /FIRE/
ERRP,IWRITE,ICY,IICY,IREDO,IREG,NHOLD,IHOLD,ITEK,
     1              IDUMP
      IREDO=0
      ISTAY=0
      J=1
      DO 400 I=1,NP
      IF (KI(I).EQ.0) GO TO 400
      IF (DABS(PD(J)/P(I)).GT.1.0D-8) ISTAY=1
      J=J+1
      IF (ICY.EQ.0) GO TO 400
      DERRP=ERRP(I)
      IF (DERRP.LE.1.0D1) GO TO 400
      IF (IREDO.EQ.0) GO TO 100
      IF (DERRP.LE.ERRP(IREDO)) GO TO 400
  100 CONTINUE
      IF (NHOLD.EQ.0) GO TO 300
      DO 200 K=1,NHOLD
      IF (I.EQ.IHOLD(K)) GO TO 400
  200 CONTINUE
```

```
  300 CONTINUE
      IREDO=I
  400 CONTINUE
      IF (ISTAY.EQ.1) GO TO 500
      ISTOP=1
  500 RETURN
      END
      SUBROUTINE MINV(N,NFAIL)
      IMPLICIT REAL*8(A-H,O-Z)
      CHARACTER*23 DATE2
C
-----------------------------------------------------------------
C
C       PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL

C        DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C        MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------
      DIMENSION AM(IP8)
      COMMON /LAND/ AM
      DATA UNDER/-300.0D0/
      CALL TIMELY(DATE2)
      WRITE (6,2100)DATE2
C     ********** SEGMENT 1 OF CHOLESKI INVERSION **********
C     ***** FACTOR MATRIX INTO LOWER TRIANGLE X TRANSPOSE *****
      K=1
      IF (N-1) 100,200,300
  100 NFAIL=K
      GO TO 2000
  200 AM(1)=1.0/AM(1)
      GO TO 1900
C     ***** LOOP M OF A(L,M) *****
  300 DO 1200 M=1,N
      IMAX=M-1
C     ***** LOOP L OF A(L,M) *****
      DO 1100 L=M,N
      SUMA=0.0
      KLI=L
      KMI=M
      IF (IMAX) 600,600,400
C     *****SUM OVER I=1,M-1 A(L,I)*A(M,I) *****
  400 DO 500 I=1,IMAX
      IF((AM(KLI).EQ.0.0D0).OR.(AM(KMI).EQ.0.0D0))  GO TO 450
      IF(DLOG10(DABS(AM(KLI)))+DLOG10(DABS(AM(KMI))).LT.UNDER)
     1      GO TO 450
```

```
      SUMA=SUMA+AM(KLI)*AM(KMI)
  450 CONTINUE
      J=N-I
      KLI=KLI+J
  500 KMI=KMI+J
C     *****TERM=C(L,M)-SUM *****
  600 TERM=AM(K)-SUMA
      IF (L-M) 700,700,1000
  700 IF (TERM) 900,900,800
C     ***** A(M,M)=SQRT(TERM) *****
  800 DENOM=DSQRT(TERM)
      AM(K)=DENOM
      GO TO 1100
  900 NFAIL=K
      GO TO 2000
C     ***** A(L,M)=TERM/A(M,M) *****
 1000 AM(K)=TERM/DENOM
 1100 K=K+1
 1200 CONTINUE
C     ********** SEGMENT 2 OF CHOLESKI INVERSION **********
C     *****INVERSION OF TRIANGULAR MATRIX*****
      AM(1)=1.0/AM(1)
      KDM=1
C     ***** STEP L OF B(L,M) *****
      DO 1500 L=2,N
      KDM=KDM+N-L+2
C     ***** RECIPROCAL OF DIAGONAL TERM *****
      TERM=1.0/AM(KDM)
      AM(KDM)=TERM
      KMI=0
      KLI=L
      IMAX=L-1
C     ***** STEP M OF B(L,M) *****
      DO 1400 M=1,IMAX
      K=KLI
C     ***** SUM TERMS *****
      SUMA=0.0
      DO 1300 I=M,IMAX
      II=KMI+I
      IF((AM(KLI).EQ.0.0D0).OR.(AM(II).EQ.0.0D0))  GO TO 1250
      IF(DLOG10(DABS(AM(KLI)))+DLOG10(DABS(AM(II))).LT.UNDER)
     1     GO TO 1250
      SUMA=SUMA-AM(KLI)*AM(II)
 1250 CONTINUE
 1300 KLI=KLI+N-I
C     ***** MULT SUM * RECIP OF DIAGONAL *****
      AM(K)=SUMA*TERM
      J=N-M
      KLI=K+J
 1400 KMI=KMI+J
 1500 CONTINUE
C     ********** SEGMENT 3 OF CHOLESKI INVERSION **********
C     *****PREMULTIPLY LOWER TRIANGLE BY TRANSPOSE*****
      K=1
```

```
      DO 1800 M=1,N
      KLI=K
      DO 1700 L=M,N
      KMI=K
      IMAX=N-L+1
      SUMA=0.0
      DO 1600 I=1,IMAX
      IF((AM(KLI).EQ.0.0D0).OR.(AM(KMI).EQ.0.0D0))  GO TO 1550
      IF(DLOG10(DABS(AM(KLI)))+DLOG10(DABS(AM(KMI))).LT.UNDER)
     1     GO TO 1550
      SUMA=SUMA+AM(KLI)*AM(KMI)
 1550 CONTINUE
      KLI=KLI+1
 1600 KMI=KMI+1
      AM(K)=SUMA
 1700 K=K+1
 1800 CONTINUE
 1900 NFAIL=0
      CALL TIMELY(DATE2)
      WRITE (6,2200)DATE2
 2000 RETURN
 2100 FORMAT(' ENTERING MATRIX INVERTER AT ^G^G^G',A23)
 2200 FORMAT(' LEAVING THE MATRIX INVERTER AT ^G^G^G',A23)
      END
      SUBROUTINE EAFW (YC,I,J)
C
-----------------------------------------------------------------
C
C                                   EAFW
C
C     "EAFW" SERVES AS A 'TRAFFIC COP' IN THAT IT DIRECTS THE FLOW
OF
C       THE CALCULATION TO THE CORRECT SUBROUTINE AS INDICATED BY
THE
C        VECTOR "IGO(J)".
C
C     LAST REVISED 1 DEC 1988 BY HAAS.
C
-----------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
      CHARACTER*1 BCD,LABEL
      CHARACTER*8 PNAME,TITLE,REF,RECKON,UNITS,YESNO,TYPE,ASTAR
C
-----------------------------------------------------------------
C
C       PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL

C         DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C         MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C        ALSO.
```

```
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------------
      DIMENSION COEF(IP4,IP3),TINV(IP4,IP3,IP10),NPHASE(IP3),
                1
IKOUNT(IP3),IGO(IP3),ISTATE(IP4,IP3),INSTAT(IP4,IP3),
     2          INVPH(IP4,IP3,IP11),INVSC(IP4,IP3),ISPECL(IP4,IP3),

     3            IPHASE(IP4,IP3),NINVER(IP4,IP3)
                        D    I    M    E    N    S    I    O    N
X(NX,IP2),P(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1          ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION ERRP(IP6),IHOLD(IP1),ITEK(4)
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION DYDC(NCPARM),DHDC(NCPARM),DGDC(NCPARM),DLYDC(2),
     1            DLHDC(2),DLGDC(2)
      DIMENSION PNAME(IP1),TITLE(10),REF(20,IP3),UNITS(4),YESNO(2),

     1            TYPE(IP9),LABEL(50)
      COMMON /EARTH/ COEF,TINV,NPHASE,IKOUNT,IGO,ISTATE,INSTAT,
     1                INVPH,INVSC,ISPECL,IPHASE,NINVER,NSETS,LISTP
      COMMON /AIR/ X,P,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1               ISING,ISTOP,IL,JDF,ION
                      C   O   M   M   O   N      /   F   I   R   E   /
ERRP,IWRITE,ICY,IICY,IREDO,IREG,NHOLD,IHOLD,ITEK,
     1                IDUMP
                     C   O   M   M   O   N      /   W   A   T   E   R   /
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1                 STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /SPACE/ DYDC,DHDC,DGDC,DLYDC,DLHDC,DLGDC,SC,TO,PT
      COMMON /HOTAIR/ PNAME,TITLE,REF,UNITS,RECKON,YESNO,ASTAR,
     1                  TYPE,LABEL,BCD
C
-----------------------------------------------------------------------
C     DETERMINE J BY LOCATING I IN THE VECTOR IKOUNT.  IF NOT
C          LOCATED, PRINT ERROR MESSAGE AND STOP
C
-----------------------------------------------------------------------
      DO 100 J=1,NSETS
      IF (I.LE.IKOUNT(J)) GO TO 200
  100 CONTINUE
      WRITE (60,60)
      STOP
  200 CONTINUE
C
-----------------------------------------------------------------------
C     WRITE REFERENCE IF THE I-TH OBSERVATION IS THE FIRST IN THE
C          J-TH DATA SET.
C
-----------------------------------------------------------------------
      IF ((IWRITE.EQ.1).OR.(I.EQ.1))  GO TO 300
      GO TO 400
```

```
  300 CONTINUE
      IF(IDUMP.LE.60)  WRITE (IDUMP,61) J,(REF(II,J),II=1,15)
      IWRITE=0
  400 CONTINUE
      JDFLAG=JDF
      IF (I.EQ.IKOUNT(J)) IWRITE=1
C
------------------------------------------------------------------
C     USING THE VECTOR IGO(J), DIRECT THE FLOW OF THE CALCULATION
TO
C          THE APPROPRIATE ROUTINE.  THEN RETURN TO THE CALLING
PROGRAM.
C
------------------------------------------------------------------
      IF(IGO(J).GT.8)  GO TO 500
      TO=X(2,I)
      IF(TO.EQ.0.D0)  TO=TREF
      PT=X(3,I)
      IF(PT.EQ.0.D0)  PT=PREF
      YC=FNCALC(X(1,I),J,IGO(J))
      GO TO 2000
  500 CONTINUE
      YC=0.D0
      IF(IGO(J).GT.9)  GO TO 600
      CALL MISCFN(YC,I,J,JDFLAG)
      GO TO 2000
  600 CONTINUE
      IF(IGO(J).GT.10)  GO TO 700
      CALL TCFIT(YC,I,J)
      GO TO 2000
  700 CONTINUE
      IF(IGO(J).GT.22)  GO TO 800
      CALL VOLUME(YC,I,J,JDFLAG)
      GO TO 2000
  800 CONTINUE
      IF(IGO(J).GT.25)  GO TO 900
      CALL MISCFN(YC,I,J,JDFLAG)
      GO TO 2000
  900 CONTINUE
      IF(IGO(J).GT.26)  GO TO 1000
      CALL DPDT(YC,I,J,JDFLAG)
      GO TO 2000
 1000 CONTINUE
      IF(IGO(J).LT.100)  GO TO 1100
      CALL UNIQUE(YC,I,J,JDFLAG)
      GO TO 2000
 1100 CONTINUE
      WRITE (60,62)IGO(J)
      STOP
C
------------------------------------------------------------------
C     RETURN
C
------------------------------------------------------------------
```

```
 2000 CONTINUE
      RETURN
C
-------------------------------------------------------------------
C     FORMAT STATEMENTS
C
-------------------------------------------------------------------
   60 FORMAT (60H0IN EAFW  I IS GREATER THAN NO, THE NUMBER OF
OBSERVAT
     1IONS./64H THEREFORE, I (THE COMPUTER) AM QUITTING. THE
PROBLEM IS
     2YOURS. )
   61 FORMAT (1H0,I5,3X,15A8/1H )
   62 FORMAT ('0IGO(J) HAS A VALUE OF ',I5,', BUT THAT DOES NOT
LEAD TO
     1A PROGRAMMED ROUTINE.'/' CHECK THE VALUE OF IGO(J).')
C
-------------------------------------------------------------------
      END
      FUNCTION FNCALC(T,J,ICODE)
C
-------------------------------------------------------------------
C
C      "FNCALC" CALCULATES THE THERMAL PROPERTIES OF A PHASE OR
SERIES OF
C       PHASES IN A CHEMICAL REACTION.  THE ROUTINE CONTAINS CODE
THAT
C        ALLOWS FOR THE FOLLOWING:
C           1.  ENTHALPY OF A REFERENCE PHASE IS 0.0 AT TREF.
C           2.  GIBBS ENERGY DIFFERENCE IS ZERO FOR TWO PHASES AT
THE
C               TRANSITION TEMPERATURE.
C                3.  ENERGY EFFECTS ASSOCIATED WITH LAMBDA-TYPE
ANOMALIES
C               ARE ACCOUNTED FOR.
C
C     LAST REVISED 1 DEC 1988 BY HAAS.
C
-------------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL*1 LAMBDA,NOLAM,UNDAMP
      CHARACTER*1 BCD,LABEL
      CHARACTER*8 PNAME,TITLE,REF,RECKON,UNITS,YESNO,TYPE,ASTAR
C
-------------------------------------------------------------------
C
C      PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL

C        DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C        MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
```

```
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------------
      DIMENSION SGN(2)
      DIMENSION COEF(IP4,IP3),TINV(IP4,IP3,IP10),NPHASE(IP3),
               1
IKOUNT(IP3),IGO(IP3),ISTATE(IP4,IP3),INSTAT(IP4,IP3),
     2          INVPH(IP4,IP3,IP11),INVSC(IP4,IP3),ISPECL(IP4,IP3),

     3            IPHASE(IP4,IP3),NINVER(IP4,IP3)
                              D    I    M    E    N    S    I    O    N
X(NX,IP2),P(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1            ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION ERRP(IP6),IHOLD(IP1),ITEK(4)
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION DYDC(NCPARM),DHDC(NCPARM),DGDC(NCPARM),DLYDC(2),
     1            DLHDC(2),DLGDC(2)
      DIMENSION LAMBDA(IP1),NOLAM(IP4,IP3)
      DIMENSION PNAME(IP1),TITLE(10),REF(20,IP3),UNITS(4),YESNO(2),

     1            TYPE(IP9),LABEL(50)
      COMMON /EARTH/ COEF,TINV,NPHASE,IKOUNT,IGO,ISTATE,INSTAT,
     1                INVPH,INVSC,ISPECL,IPHASE,NINVER,NSETS,LISTP
      COMMON /AIR/ X,P,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1               ISING,ISTOP,IL,JDF,ION
                      C   O   M   M   O   N       /   F   I   R   E   /
ERRP,IWRITE,ICY,IICY,IREDO,IREG,NHOLD,IHOLD,ITEK,
     1                IDUMP
                      C   O   M   M   O   N       /   W   A   T   E   R   /
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1                 STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /SPACE/ DYDC,DHDC,DGDC,DLYDC,DLHDC,DLGDC,SC,TO,PT
      COMMON /AETHER/ LAMBDA,NOLAM,UNDAMP
      COMMON /HOTAIR/ PNAME,TITLE,REF,UNITS,RECKON,YESNO,ASTAR,
     1                  TYPE,LABEL,BCD
C
-----------------------------------------------------------------------
C     INITIALIZE VARIABLES
C
-----------------------------------------------------------------------
      FNCALC=ZERO
      DO 100 K=1,NP
      DC(K)=ZERO
  100 CONTINUE
      LAST=NPHASE(J)
C
-----------------------------------------------------------------------
C        FOR  EACH  PHASE  IN  THE  J-TH  DATA  SET,  CALCULATE  THE
DERIVATIVES
C        "DC" FOR EACH CONSTANT.
C
```

```
------------------------------------------------------------------------
      DO 1700 L=1,LAST
C
------------------------------------------------------------------------
C     LOCATE THE FIRST CONSTANT FOR THE L-TH PHASE IN THE VECTOR P.

C        INITIALIZE SC, THE STOICHIOMETRIC COEFFICIENT.
C
------------------------------------------------------------------------
      INDEX=1+NPARM*(IPHASE(L,J)-1)
      SC=COEF(L,J)
C
------------------------------------------------------------------------
C     IF THE PHASE HAS A LAMBDA TRANSITION, SET THE PARAMETER TC
C
------------------------------------------------------------------------
      TC=P(INDEX+NCPARM)*(0.1d0*P(INDEX+NCPARM+1)*(PT-PREF)+1.D0)
C
------------------------------------------------------------------------
C        CALL  YDERIV  TO  CALCULATE  THE  TEMPERATURE  TERM  IN  THE
DERIVATIVE.
C        IF THE DATA SET IS FOR ENTROPY AND HEAT CAPACITY,  GO TO
C        STATEMENT 1400.
C
------------------------------------------------------------------------
      IGOES=ICODE
      IF (ISTATE(L,J).EQ.-1) IGOES=IGOES+7
      CALL YDERIV(T,IGOES)
      IF(ISPECL(L,J).EQ.-1)  CALL YDERIV(TO,IGOES)
      IF (ICODE.LE.2) GO TO 1400
C
------------------------------------------------------------------------
C     CALL HDERIV TO CALCULATE THE DERIVATIVE WITH RESPECT TO "A9"
AT
C       298.15 KELVIN IF SPECIES IS AN ELEMENT.  PROCEED TO ADJUST

C        DC ACCORDINGLY
C
------------------------------------------------------------------------
      IF (ISTATE(L,J).NE.1) GO TO 300
      CALL HDERIV(TREF)
      DO 200 K=1,NCPARM
      DC(K+INDEX-1)=DC(K+INDEX-1)+SC*DHDC(K)*DYDC(9)
  200 CONTINUE
      IF(NOLAM(L,J))  GO TO 220
      IF(.NOT.LAMBDA(IPHASE(L,J))) GO TO 220
      JL=P(INDEX+NCPARM+NMPARM+NVPARM)
      JH=P(INDEX+NCPARM+NMPARM+NVPARM+1)
      JT=P(INDEX+NCPARM+NMPARM+NVPARM+2)
      CALL LHDRIV(TREF,INDEX,JL,JH,JT)
      DC(INDEX+NCPARM+2)=DC(INDEX+NCPARM+2)+SC*DYDC(9)*DLHDC(1)
      IF(TREF.LE.TC)  GO TO 220
      DC(INDEX+NCPARM+3)=DC(INDEX+NCPARM+3)+SC*DYDC(9)*DLHDC(2)
  220 CONTINUE
```

```
      GO TO 1400
  300 CONTINUE
C
---------------------------------------------------------------------
C     CHECK FOR INVERSIONS.  IF LOW TEMPERATURE PHASES ARE TO BE
C        CONSIDERED, INITIALIZE SGN.  IF LOW TEMPERATURE PHASES
C        ARE NOT TO BE CONSIDERED, GO TO STATEMENT 1400 BELOW
C
---------------------------------------------------------------------
      IF (NINVER(L,J).LE.0) GO TO 1400
      DO 400 LLL=1,2
      SGN(LLL)=SCINV(LLL)
  400 CONTINUE
      IF (INVSC(L,J).EQ.0) GO TO 500
      SGN(1)=SGN(1)*STCOEF(INVSC(L,J))
      SGN(2)=SGN(2)*STCOEF(INVSC(L,J))
  500 CONTINUE
C
---------------------------------------------------------------------
C    IF THE LOWEST TEMPERATURE PHASE IS AN ELEMENT, CALL "HDERIV".

C       THE ARGUMENT IS 298.15.  PROCEED TO ADJUST DC ACCORDINGLY.

C
---------------------------------------------------------------------
      IF (INSTAT(L,J).EQ.0) GO TO 800
      IINVR=1+NPARM*(INVPH(L,J,1)-1)
      CALL HDERIV(TREF)
      DO 600 K=1,NCPARM
      DC(K+IINVR-1)=DC(K+IINVR-1)+DHDC(K)*SGN(2)*SC*DYDC(9)
  600 CONTINUE
      IF(.NOT.LAMBDA(INVPH(L,J,1)))  GO TO 700
      JL=P(IINVR+NCPARM+NMPARM+NVPARM)
      JH=P(IINVR+NCPARM+NMPARM+NVPARM+1)
      JT=P(IINVR+NCPARM+NMPARM+NVPARM+2)
      CALL LHDRIV(TREF,IINVR,JL,JH,JT)

DC(IINVR+NCPARM+2)=DC(IINVR+NCPARM+2)+SC*SGN(2)*DYDC(9)*DLHDC(1)
      IF(TREF.LE.TC)  GO TO 700

DC(IINVR+NCPARM+3)=DC(IINVR+NCPARM+3)+SC*SGN(2)*DYDC(9)*DLHDC(2)
  700 CONTINUE
  800 CONTINUE
C
---------------------------------------------------------------------
C    CALL GDERIV TO CALCULATE THE DERIVATIVE WITH RESPECT TO "A9"
FOR
C        HIGH AND LOW TEMPERATURE PHASE AT TEMPERATURE OF
C        INVERSION.  PROCEED TO ADJUST DC ACCORDINGLY
C
---------------------------------------------------------------------
      LSTINV=NINVER(L,J)
      DO 1300 LL=1,LSTINV
      CALL GDERIV(TINV(L,J,LL))
```

```
C
----------------------------------------------------------------
C    IF THERE IS A STOICHIOMETRY CHANGE FOR THE HIGHEST TRANSITION

C        (EG: 2 FECL2(L) = FE2CL4(G)), ADJUST SGN(2) ACCORDINGLY
C
----------------------------------------------------------------
      IF (INVSC(L,J).EQ.0) GO TO 900
      IF (LL.NE.LSTINV) GO TO 900
      SGN(2)=SGN(2)/STCOEF(INVSC(L,J))
  900 CONTINUE
      DO 1200 LLL=1,2
      IINVR=1+NPARM*(INVPH(L,J,(LL+LLL-1))-1)
      DO 1000 K=1,NCPARM
      DC(K+IINVR-1)=DC(K+IINVR-1)+DGDC(K)*SGN(LLL)*SC*DYDC(9)
 1000 CONTINUE
      IF(.NOT.LAMBDA(INVPH(L,J,(LL+LLL-1)))) GO TO 1100
      JL=P(IINVR+NCPARM+NMPARM+NVPARM)
      JH=P(IINVR+NCPARM+NMPARM+NVPARM+1)
      JT=P(IINVR+NCPARM+NMPARM+NVPARM+2)
      TINVER=TINV(L,J,LL)
      CALL LGDRIV(TINVER,IINVR,JL,JH,JT)

DC(IINVR+NCPARM+2)=DC(IINVR+NCPARM+2)+SC*SGN(LLL)*DYDC(9)*DLGDC(1)
      IF(TINVER.LE.TC)  GO TO 1100

DC(IINVR+NCPARM+3)=DC(IINVR+NCPARM+3)+SC*SGN(LLL)*DYDC(9)*DLGDC(2)
 1100 CONTINUE
 1200 CONTINUE
 1300 CONTINUE
 1400 CONTINUE
C
----------------------------------------------------------------
C     COMPLETE THE CALCULATION OF DC BY ADDING THE DERIVATIVE AT
T(OBS).
C
----------------------------------------------------------------
      DO 1500 K=1,NCPARM
      DC(K+INDEX-1)=DC(K+INDEX-1)+SC*DYDC(K)
 1500 CONTINUE
C
----------------------------------------------------------------
C     COMPLETE WITH THE CALCULATION AT T(CRIT) IF APPLICABLE.
C
----------------------------------------------------------------
      IF(NOLAM(L,J))  GO TO 1600
      IF(.NOT.LAMBDA(IPHASE(L,J))) GO TO 1600
      JL=P(INDEX+NCPARM+NMPARM+NVPARM)
      JH=P(INDEX+NCPARM+NMPARM+NVPARM+1)
      JT=P(INDEX+NCPARM+NMPARM+NVPARM+2)
      CALL LYDRIV(T,IGOES,INDEX,JL,JH,JT)
      DC(INDEX+NCPARM+2)=DC(INDEX+NCPARM+2)+SC*DLYDC(1)
      IF(T.LE.TC)  GO TO 1600
      DC(INDEX+NCPARM+3)=DC(INDEX+NCPARM+3)+SC*DLYDC(2)
```

```
 1600 CONTINUE
 1700 CONTINUE
C
-----------------------------------------------------------------------
C     ALL DERIVATIVES HAVE BEEN CALCULATED.  NOW CALCULATE FNCALC
BY
C        SUMMING THE PRODUCT DC*P.  ADD IN THE COMPONENT DUE TO
C        THE LAMBDA ANOMALY IF APPROPRIATE.
C
-----------------------------------------------------------------------
      DO 1800 K=1,NP
      IF(MOD(K,NPARM).EQ.NCPARM+1)  GO TO 1800
      IF(MOD(K,NPARM).EQ.NCPARM+2)  GO TO 1800
      FNCALC=FNCALC+P(K)*DC(K)
 1800 CONTINUE
C
-----------------------------------------------------------------------
C     RETURN TO THE CALLING PROGRAM
C
-----------------------------------------------------------------------
      RETURN
      END
      SUBROUTINE VOLUME(Y,I,J,JDFLAG)
C
-----------------------------------------------------------------------
C
C      "VOLUME" IS DESIGNED TO CALCULATE VOLUME-RELATED FUNCTIONS
FOR A
C       PHASE OR A GROUP OF PHASES.  THE FUNCTIONS ARE AS FOLLOWS:

C       IGO(J)     FUNCTION
C         11       V(T,P), MOLAR VOLUME.
C         12       V(T,P), CELL VOLUME.
C         13       V-VO, VOLUME RELATIVE TO A REFERENCE VOLUME.
C         14       V/VO, REDUCED VOLUME.
C         15       ALPHA, CUBIC EXPANSION COEFFICIENT.
C         16       (V-VO)/VO AT CONSTANT PRESSURE.
C         17       (V-VO)/[VO*(T-TO)] AT CONSTANT PRESSURE.
C         18       KAPPA-T(T,P), ISOTHERMAL COMPRESSIBILITY.
C         19       B-T(T,P), ISOTHERMAL BULK MODULUS.
C         20       (V-VO)/VO AT CONSTANT TEMPERATURE.
C         21       (V-VO)/[VO*(P-PO)] AT CONSTANT TEMPERATURE.
C        22      G(T,P) AND DELTA G(T,P), GIBBS ENERGY AT ELEVATED
C                    TEMPERATURE AND PRESSURE.
C
C     LAST REVISED 1 DEC 1988 BY HAAS.
C
-----------------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL*1 LAMBDA,NOLAM,UNDAMP
      CHARACTER*1 BCD,LABEL
      CHARACTER*8 PNAME,TITLE,REF,RECKON,UNITS,YESNO,TYPE,ASTAR
      REAL*8 KBM,KBMO,INTVDP
C
```

```
-----------------------------------------------------------------
C
C       PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C         IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL

C         DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C         MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C         ALSO.
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------
      DIMENSION COEF(IP4,IP3),TINV(IP4,IP3,IP10),NPHASE(IP3),
               1
IKOUNT(IP3),IGO(IP3),ISTATE(IP4,IP3),INSTAT(IP4,IP3),
     2        INVPH(IP4,IP3,IP11),INVSC(IP4,IP3),ISPECL(IP4,IP3),

     3          IPHASE(IP4,IP3),NINVER(IP4,IP3)
                               DIMENSION
X(NX,IP2),PC(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1          ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION DYDC(NCPARM),DHDC(NCPARM),DGDC(NCPARM),DLYDC(2),
     1          DLHDC(2),DLGDC(2)
      DIMENSION LAMBDA(IP1),NOLAM(IP4,IP3)
      DIMENSION PNAME(IP1),TITLE(10),REF(20,IP3),UNITS(4),YESNO(2),

     1          TYPE(IP9),LABEL(50)
      COMMON /EARTH/ COEF,TINV,NPHASE,IKOUNT,IGO,ISTATE,INSTAT,
     1              INVPH,INVSC,ISPECL,IPHASE,NINVER,NSETS,LISTP
      COMMON/AIR/X,PC,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1             ISING,ISTOP,IL,JDF,ION
                        COMMON                /WATER/
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1              STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /SPACE/ DYDC,DHDC,DGDC,DLYDC,DLHDC,DLGDC,SC,TO,PT
      COMMON /AETHER/ LAMBDA,NOLAM,UNDAMP
      COMMON /HOTAIR/ PNAME,TITLE,REF,UNITS,RECKON,YESNO,ASTAR,
     1               TYPE,LABEL,BCD
C
-----------------------------------------------------------------
C    INITIALIZE CONSTANTS.  IF NOTSPECIFIED, "TO" IS SET TO "TREF"
AND
C         "P" AND "PO" ARE SET TO "PREF".
C
-----------------------------------------------------------------
      DO 100 N=1,NP
      DC(N)=0.0D0
  100 CONTINUE
      Y=0.0D0
```

```
      T=X(1,I)
      TO=X(2,I)
      IF(TO.NE.0.0D0)  GO TO 200
      TO=TREF
      X(2,I)=TREF
  200 CONTINUE
      P=X(3,I)
      IF(P.NE.0.0D0)  GO TO 300
      P=PREF
      X(3,I)=PREF
  300 CONTINUE
      PO=X(4,I)
      IF(PO.NE.0.0D0)  GO TO 400
      PO=PREF
      X(4,I)=PREF
  400 CONTINUE
      LAST=NPHASE(J)
      IGOES=IGO(J)-10
      PT=PREF
      IF(IGOES.EQ.12)  Y=FNCALC(X(1,I),J,4)
      IF(IGOES.NE.4)  GO TO 500
      IF(LAST.EQ.2)  GO TO 9000
  500 CONTINUE
      DO 8900 L=1,LAST
      ACOEF=COEF(L,J)
      INDEX=1+NPARM*(IPHASE(L,J)-1)
      IT=INDEX+NCPARM+NMPARM
      B1=PC(IT)
      B2=PC(IT+1)
      B3=PC(IT+2)
      B4=PC(IT+3)
      B5=PC(IT+4)
      B6=PC(IT+5)
      VR=PC(IT+6)
      DEBT=PC(IT+7)
      RTT=DEXP(-T/DEBT)
      RTTO=DEXP(-TO/DEBT)
      IF(NOLAM(L,J))  GO TO 600
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 600
      A12=PC(IT-3)
      TC=PC(IT-4)*(0.1d0*PC(IT-3)*(P-PREF)+ONE)
      TCO=PC(IT-4)*(0.1D0*PC(IT-3)*(PO-PREF)+ONE)
      PT=P
      A13=PC(IT-2)
      A14=PC(IT-1)
      TAU=T/TC
      TAUO=TO/TCO
      JL=PC(IT+8)
      JH=PC(IT+9)
      JT=PC(IT+10)
  600 CONTINUE
                                              GO TO
(1000,1000,2000,3000,4000,5000,5000,6000,6000,7000,7000,
     1       8000,9990), IGOES
```

```
C
-----------------------------------------------------------------
C     V(MOLAR) = [B7*DEXP("Z")+V(M)]*[1+B6*P/(B4+B5*T)]**-(1/B6)
C
C     AND V(CELL) = V(MOLAR)*X(5,I)/A
C
C
C        WHERE "Z" = B1*T + B2*T**2/2 - B8*B3*DEXP(-T/B8)
C        V(M) = A12*H(M),
C        A = AVOGADRO CONSTANT,
C        AND X(5,I) = NUMBER OF FORMULA UNITS IN THE UNIT CELL.
C
C     V(MOLAR) IS GIVEN IN CM**3/MOL AND V(CELL) IS GIVEN IN
C        ANGSTROM**3/UNIT CELL.
C
C     FOR DATA MEASURED AT PREF OR LESS, "P" IS SET TO 0.0D0.  THE
SAME
C        ALSO HOLDS FOR "PO".
C
-----------------------------------------------------------------
 1000 CONTINUE
      FACT=1.D0
      IF(IGO(J).EQ.12)  FACT=X(5,I)/A
      ACOEF=ACOEF*FACT
      IF(P.LE.PREF)  P=0.D0
      KBM=B4+B5*T
      U=ONE+B6*P/KBM
      W=-ONE/B6
      UW=U**W
      Z=B1*T+B2*T*T/TWO-DEBT*B3*RTT
      VRZ=VR*DEXP(Z)
      VT=VRZ
      IF(NOLAM(L,J))  GO TO 1100
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 1100
      CALL LYDRIV(T,3,INDEX,JL,JH,JT)
      VT=VT+A12*A13*DLYDC(1)
      DC(IT-2)=DC(IT-2)+ACOEF*UW*A12*DLYDC(1)
      DC(IT-3)=DC(IT-3)+ACOEF*UW*A13*DLYDC(1)
      IF(TAU.LE.ONE)  GO TO 1100
      VT=VT+A12*A14*DLYDC(2)
      DC(IT-1)=DC(IT-1)+ACOEF*UW*A12*DLYDC(2)
      DC(IT-3)=DC(IT-3)+ACOEF*UW*A14*DLYDC(2)
 1100 CONTINUE
      Y=Y+ACOEF*VT*UW
      IF(JDFLAG.NE.0)  GO TO 8900
      DUDB4=-B6*P/KBM**2
      DUDB5=DUDB4*T
      DUDB6=P/KBM
      DWDB6=B6**(-2)
      WUWL1=W*U**(W-ONE)
      DC(IT)=DC(IT)+ACOEF*UW*VRZ*T
      DC(IT+1)=DC(IT+1)+ACOEF*UW*VRZ*T*T/TWO
      DC(IT+2)=DC(IT+2)-ACOEF*UW*VRZ*DEBT*RTT
      DC(IT+3)=DC(IT+3)+ACOEF*VT*WUWL1*DUDB4
```

```
      DC(IT+4)=DC(IT+4)+ACOEF*VT*WUWL1*DUDB5
      DC(IT+5)=DC(IT+5)+ACOEF*VT*
     1     (WUWL1*DUDB6+UW*DLOG(U)*DWDB6)
      DC(IT+6)=DC(IT+6)+ACOEF*UW*DEXP(Z)
      GO TO 8900
C
----------------------------------------------------------------
C     V-VO = [V EVALUATED AT (T,P)] - [VO EVALUATED AT (TO,PO)].
C
C     THE PHASES AT (T,P) AND AT (TO,PO) MAY BE THE SAME OR MAY BE
C          DIFFERENT.  FOR PROPER CALCULATION, TWO OR MORE PHASES
MUST
C         BE ENTERED.  THE PHASES WITH A STOICHIOMETRIC COEFFICIENT
OF
C         '-' WILL BE EVALUATED AT (TO,PO).
C     FOR DATA MEASURED AT PREF OR LESS, "P" IS SET TO 0.0D0.  THE
SAME
C         ALSO HOLDS FOR "PO".
C
----------------------------------------------------------------
 2000 CONTINUE
      IF(P.LE.PREF)  P=0.D0
      IF(ACOEF.LT.ZERO)  GO TO 2200
      KBM=B4+B5*T
      U=ONE+B6*P/KBM
      W=-ONE/B6
      UW=U**W
      Z=B1*T+B2*T*T/TWO-DEBT*B3*RTT
      VRZ=VR*DEXP(Z)
      VT=VRZ
      IF(NOLAM(L,J))  GO TO 2100
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 2100
      CALL LYDRIV(T,3,INDEX,JL,JH,JT)
      VT=VT+A12*A13*DLYDC(1)
      DC(IT-2)=DC(IT-2)+ACOEF*UW*A12*DLYDC(1)
      DC(IT-3)=DC(IT-3)+ACOEF*UW*A13*DLYDC(1)
      IF(TAU.LE.ONE)  GO TO 2100
      VT=VT+A12*A14*DLYDC(2)
      DC(IT-1)=DC(IT-1)+ACOEF*UW*A12*DLYDC(2)
      DC(IT-3)=DC(IT-3)+ACOEF*UW*A14*DLYDC(2)
 2100 CONTINUE
      Y=Y+ACOEF*VT*UW
      IF(JDFLAG.NE.0)  GO TO 8900
      DUDB4=-B6*P/KBM**2
      DUDB5=DUDB4*T
      DUDB6=P/KBM
      DWDB6=B6**(-2)
      WUWL1=W*U**(W-ONE)
      DC(IT)=DC(IT)+ACOEF*UW*VRZ*T
      DC(IT+1)=DC(IT+1)+ACOEF*UW*VRZ*T*T/TWO
      DC(IT+2)=DC(IT+2)-ACOEF*UW*VRZ*DEBT*RTT
      DC(IT+3)=DC(IT+3)+ACOEF*VT*WUWL1*DUDB4
      DC(IT+4)=DC(IT+4)+ACOEF*VT*WUWL1*DUDB5
      DC(IT+5)=DC(IT+5)+ACOEF*VT*
```

```
     1     (WUWL1*DUDB6+UW*DLOG(U)*DWDB6)
      DC(IT+6)=DC(IT+6)+ACOEF*UW*DEXP(Z)
      GO TO 8900
 2200 CONTINUE
      IF(PO.LE.PREF)  PO=0.D0
      KBMO=B4+B5*TO
      UO=ONE+B6*PO/(KBMO)
      W=-ONE/B6
      UOW=UO**W
      ZO=B1*TO+B2*TO*TO/TWO-DEBT*B3*RTTO
      VRZO=VR*DEXP(ZO)
      VTO=VRZO
      IF(NOLAM(L,J))  GO TO 2300
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 2300
      PT=PO
      CALL LYDRIV(TO,3,INDEX,JL,JH,JT)
      VTO=VTO+A12*A13*DLYDC(1)
      DC(IT-2)=DC(IT-2)+ACOEF*UOW*A12*DLYDC(1)
      DC(IT-3)=DC(IT-3)+ACOEF*UOW*A13*DLYDC(1)
      IF(TAUO.LE.ONE)  GO TO 2300
      VTO=VTO+A12*A14*DLYDC(2)
      DC(IT-1)=DC(IT-1)+ACOEF*UOW*A12*DLYDC(2)
      DC(IT-3)=DC(IT-3)+ACOEF*UOW*A14*DLYDC(2)
 2300 CONTINUE
      Y=Y+ACOEF*VTO*UOW
      IF(JDFLAG.NE.0)  GO TO 8900
      DUDB4=-B6*PO/KBMO**2
      DUDB5=DUDB4*TO
      DUDB6=PO/KBMO
      DWDB6=B6**(-2)
      WUOWL1=W*UO**(W-ONE)
      DC(IT)=DC(IT)+ACOEF*UOW*VRZO*TO
      DC(IT+1)=DC(IT+1)+ACOEF*UOW*VRZO*TO*TO/TWO
      DC(IT+2)=DC(IT+2)-ACOEF*UOW*VRZO*DEBT*RTTO
      DC(IT+3)=DC(IT+3)+ACOEF*VT*WUOWL1*DUDB4
      DC(IT+4)=DC(IT+4)+ACOEF*VT*WUOWL1*DUDB5
      DC(IT+5)=DC(IT+5)+ACOEF*VT*
     1     (WUOWL1*DUDB6+UOW*DLOG(UO)*DWDB6)
      DC(IT+6)=DC(IT+6)+ACOEF*UOW*DEXP(ZO)
      GO TO 8900
C
-----------------------------------------------------------------
C     V/VO = [V EVALUATED AT (T,P)]/[VO EVALUATED AT (TO,PO)].
C
C    THE PHASES AT (T,P) AND AT (TO,PO) MAY BE THE SAME OR MAY BE
C        DIFFERENT.  IF 2 OR MORE PHASES ARE ENTERED, THE PHASES
WITH
C       NEGATIVE STOECHIOMETRIC COEFFICIENTS WILL BE EVALUATED AT
C       (TO,PO) AND THE PHASES WITH POSITIVE COEFFICIENTS WILL BE
C        EVALUATED AT (T,P).
C
-----------------------------------------------------------------
 3000 CONTINUE
      IF(P.LE.PREF)  P=0.D0
```

```
      IF((T.EQ.TO).AND.(PO.LE.PREF))  GO TO 3300
      KBM=B4+B5*T
      U=ONE+B6*P/KBM
      W=-ONE/B6
      UW=U**W
      Z=B1*T+B2*T*T/TWO-DEBT*B3*RTT
      VRZ=VR*DEXP(Z)
      VT=VRZ
      IF(NOLAM(L,J))  GO TO 3100
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 3100
      DLDC1=ZERO
      DLDC2=ZERO
      CALL LYDRIV(T,3,INDEX,JL,JH,JT)
      VT=VT+A12*A13*DLYDC(1)
      DLDC1=DLYDC(1)
      IF(TAU.LE.ONE)  GO TO 3100
      VT=VT+A12*A14*DLYDC(2)
      DLDC2=DLYDC(2)
3100  CONTINUE
      IF(PO.LE.PREF)  PO=ZERO
      KBMO=B4+B5*TO
      UO=ONE+B6*PO/(KBMO)
      UOW=UO**(-W)
      ZO=B1*TO+B2*TO*TO/TWO-DEBT*B3*RTTO
      VRZO=VR*DEXP(ZO)
      VTO=VRZO
      IF(NOLAM(L,J))  GO TO 3200
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 3200
      DLDC10=ZERO
      DLDC20=ZERO
      TAUO=TO/TCO
      PT=PO
      CALL LYDRIV(TO,3,INDEX,JL,JH,JT)
      VTO=VTO+A12*A13*DLYDC(1)
      DLDC10=DLYDC(1)
      IF(TAUO.LE.ONE)  GO TO 3200
      VTO=VTO+A12*A14*DLYDC(2)
      DLDC20=DLYDC(2)
3200  CONTINUE
      RV=VT/VTO
      RUW=(U/UO)**W
      Y=Y+ACOEF*RV*RUW
      IF(JDFLAG.NE.0)  GO TO 8900
      DUDB4=-B6*P/KBM**2
      DUDB5=DUDB4*T
      DUDB6=P/KBM
      DUODB4=-B6*PO/KBMO**2
      DUODB5=DUODB4*TO
      DUODB6=PO/KBMO
      DWDB6=B6**(-2)
      WUWL1=W*U**(W-ONE)
      DUWDB4=WUWL1*DUDB4
      DUWDB5=WUWL1*DUDB5
      DUWDB6=WUWL1*DUDB6+UW*DLOG(U)*DWDB6
```

```
      WUOWL1=-W*UO**(-(W+ONE))
      DUOWDB4=WUOWL1*DUODB4
      DUOWDB5=WUOWL1*DUODB5
      DUOWDB6=WUOWL1*DUODB6-UOW*DLOG(UO)*DWDB6
      RVTOSQ=1.D0/VTO**2
      DC(IT)=DC(IT)+ACOEF*RUW*(VTO*VRZ*T-VT*VRZO*TO)*RVTOSQ

DC(IT+1)=DC(IT+1)+ACOEF*RUW*(VTO*VRZ*T*T-VT*VRZO*TO*TO)*RVTOSQ/TWO

DC(IT+2)=DC(IT+2)-ACOEF*RUW*DEBT*(VTO*VRZ*RTT-VT*VRZO*RTTO)*RVTOSQ
      DC(IT+3)=DC(IT+3)+ACOEF*RV*
     1     (UW*DUOWDB4+UOW*DUWDB4)
      DC(IT+4)=DC(IT+4)+ACOEF*RV*
     1     (UW*DUOWDB5+UOW*DUWDB5)
      DC(IT+5)=DC(IT+5)+ACOEF*RV*
     1     (UW*DUOWDB6+UOW*DUWDB6)
      DC(IT+6)=DC(IT+6)+ACOEF*RUW*(VTO*DEXP(Z)-VT*DEXP(ZO))*RVTOSQ
      IF(NOLAM(L,J))  GO TO 3400
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 3400
      DC(IT-2)=DC(IT-2)+
     1           ACOEF*RUW*A12*(VTO*DLDC1-VT*DLDC10)*RVTOSQ
      DC(IT-3)=DC(IT-3)+
     1           ACOEF*RUW*A13*(VTO*DLDC1-VT*DLDC10)*RVTOSQ
      IF(TAU.LE.ONE)  GO TO 3400
      DC(IT-1)=DC(IT-1)+
     1           ACOEF*RUW*A12*(VTO*DLDC2-VT*DLDC20)*RVTOSQ
      DC(IT-3)=DC(IT-3)+
     1           ACOEF*RUW*A14*(VTO*DLDC2-VT*DLDC20)*RVTOSQ
      GO TO 3400
 3300 CONTINUE
      KBM=B4+B5*T
      U=ONE+B6*P/KBM
      W=-ONE/B6
      UW=U**W
      Y=Y+ACOEF*UW
      IF(JDFLAG.NE.0)  GO TO 8900
      DUDB4=-B6*P/KBM**2
      DUDB5=DUDB4*T
      DUDB6=P/KBM
      DWDB6=B6**(-2)
      WUWL1=W*U**(W-ONE)
C     DC(IT)=DC(IT)+ZERO
C     DC(IT+1)=DC(IT+1)+ZERO
C     DC(IT+2)=DC(IT+2)+ZERO
      DC(IT+3)=DC(IT+3)+ACOEF*WUWL1*DUDB4
      DC(IT+4)=DC(IT+4)+ACOEF*WUWL1*DUDB5
      DC(IT+5)=DC(IT+5)+ACOEF*(WUWL1*DUDB6+UW*DLOG(U)*DWDB6)
C     DC(IT+6)=DC(IT+6)+ZERO
 3400 CONTINUE
      GO TO 8900
C
-----------------------------------------------------------------
C                d                d
C     ALPHA = VO --(U**W) + U**W --(VO)
```

```
C                dT               dT
C
C        WHERE VO = THE VOLUME EVALUATED AT ZERO PRESSURE
C        [= B8*DEXP(Z)+V(M)] AND
C        U**W = [1+B6*P/(B4+B5*T)]**-(1/B6)
C
---------------------------------------------------------------
 4000 CONTINUE
      IF(P.LE.PREF)  P=0.D0
      ALPHA=B1+B2*T+B3*RTT
      DVMDT=ZERO
      IF(NOLAM(L,J))  GO TO 4200
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 4200
      CALL LYDRIV(T,1,INDEX,JL,JH,JT)
      DLDC1=DLYDC(1)
      DLDC2=DLYDC(2)
      IF(TAU.GT.ONE)  GO TO 4100
      DVMDT=DVMDT+A12*A13*DLDC1
      GO TO 4200
 4100 CONTINUE
      DVMDT=DVMDT+A12*A14*DLDC2
 4200 CONTINUE
      Z=B1*T+B2*T*T/TWO-DEBT*B3*RTT
      VRZ=VR*DEXP(Z)
      VT=VRZ
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 4300
      CALL LYDRIV(T,3,INDEX,JL,JH,JT)
      DLDC10=DLYDC(1)
      DLDC20=DLYDC(2)
      VT=VT+A12*A13*DLDC10
      IF(TAU.LE.ONE)  GO TO 4300
      VT=VT+A12*A14*DLDC20
 4300 CONTINUE
      KBM=B4+B5*T
      F1=1.D0/(KBM+B6*P)
      F2=1.D0/KBM
      Y=Y+ACOEF*(B5*P*F1*F2+(ALPHA*VRZ+DVMDT)/VT)
      IF(JDFLAG.NE.0)  GO TO 8900
      DVTDT=VRZ*ALPHA+DVMDT
      DC(IT)=DC(IT)+ACOEF*VRZ*(1.D0+ALPHA*T-DVTDT*T/VT)/VT

DC(IT+1)=DC(IT+1)+VRZ*T*(1.D0+ALPHA*T/2.D0-DVTDT*T/(2.D0*VT))/VT
      DC(IT+2)=DC(IT+2)+VRZ*RTT*(1.D0-ALPHA*DEBT+DVTDT*DEBT/VT)/VT
      DC(IT+3)=DC(IT+3)-B5*P*F1*F2*(F2+F1)
      DC(IT+4)=DC(IT+4)+F1*F2*P*(1.D0-B5*F1*T-B5*F2*T)
      DC(IT+5)=DC(IT+5)-B5*P*P*F1*F2*(F2+F1)
      DC(IT+6)=DC(IT+6)+DEXP(Z)*(ALPHA-DVTDT/VT)/VT
      IF(NOLAM(L,J))  GO TO 4400
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 4400
      DC(IT-2)=DC(IT-2)+
     1            ACOEF*A12*(DLDC1-DVMDT*DLDC10/VT)/VT
      DC(IT-3)=DC(IT-3)+
     1            ACOEF*A13*(DLDC1-DVMDT*DLDC10/VT)/VT
      IF(TAU.LE.ONE)  GO TO 4400
```

```
      DC(IT-1)=DC(IT-1)+
     1           ACOEF*A12*(DLDC2-DVMDT*DLDC20/VT)/VT
      DC(IT-3)=DC(IT-3)+
     1           ACOEF*A14*(DLDC2-DVMDT*DLDC20/VT)/VT
 4400 CONTINUE
      GO TO 8900
C
C------------------------------------------------------------------
C     YC = [V(T,P)-V(TO,P)]/[V(TO,P)*DT]
C
C        WHERE "DT" = T-TO.
C
C      THE SAME PHASE IS EVALUATED BOTH AT (T,P) AND (TO,P).  IF
"IGO(J)"
C        = 16, DT IS SET EQUAL TO 1.D0.
C
C------------------------------------------------------------------
 5000 CONTINUE
      IF(P.LE.PREF)  P=0.D0
      ZO=B1*TO+B2*TO*TO/TWO-DEBT*B3*RTTO
      VRZO=VR*DEXP(ZO)
      VTO=VRZO
      IF(NOLAM(L,J)) GO TO 5100
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 5100
      DLDC10=ZERO
      DLDC20=ZERO
      CALL LYDRIV(TO,3,INDEX,JL,JH,JT)
      VTO=VTO+A12*A13*DLYDC(1)
      DLDC10=DLYDC(1)
      IF(TAUO.LE.ONE)  GO TO 5100
      VTO=VTO+A12*A14*DLYDC(2)
      DLDC20=DLYDC(2)
 5100 CONTINUE
      Z=B1*T+B2*T*T/TWO-DEBT*B3*RTT
      VRZ=VR*DEXP(Z)
      VT=VRZ
      IF(NOLAM(L,J)) GO TO 5200
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 5200
      DLDC1=ZERO
      DLDC2=ZERO
      CALL LYDRIV(T,3,INDEX,JL,JH,JT)
      VT=VT+A12*A13*DLYDC(1)
      DLDC1=DLYDC(1)
      IF(TAU.LE.ONE)  GO TO 5200
      VT=VT+A12*A14*DLYDC(2)
      DLDC2=DLYDC(2)
 5200 CONTINUE
      DT=T-TO
      IF(IGO(J).EQ.16)  DT=ONE
      RV=VT/VTO
      KBM=B4+B5*T
      KBMO=B4+B5*TO
      U=ONE+B6*P/KBM
      UO=ONE+B6*P/KBMO
```

```
      W=-ONE/B6
      UW=U**W
      UOW=UO**(-W)
      RUW=UW*UOW
      Y=(RV*RUW-ONE)/DT
      IF(JDFLAG.NE.0)  GO TO 8900
      WUWL1=W*U**(W-ONE)
      WUOWL1=-W*UO**(-(W+ONE))
      DUDB4=-B6*P/KBM**2
      DUDB5=DUDB4*T
      DUDB6=P/KBM
      DUODB4=-B6*P/KBMO**2
      DUODB5=DUODB4*TO
      DUODB6=P/KBMO
      DWDB6=B6**(-2)
      DUWDB4=WUWL1*DUDB4
      DUWDB5=WUWL1*DUDB5
      DUWDB6=WUWL1*DUDB6+UW*DLOG(U)*DWDB6
      DUOWDB4=WUOWL1*DUODB4
      DUOWDB5=WUOWL1*DUODB5
      DUOWDB6=WUOWL1*DUODB6-UOW*DLOG(UO)*DWDB6
      RDTVTO=1.D0/(DT*VTO**2)
      DC(IT)=DC(IT)+ACOEF*RUW*(VTO*VRZ*T-VT*VRZO*TO)*RDTVTO

DC(IT+1)=DC(IT+1)+ACOEF*RUW*(VTO*VRZ*T*T-VT*VRZO*TO*TO)*RDTVTO/TWO

DC(IT+2)=DC(IT+2)-ACOEF*RUW*DEBT*(VTO*VRZ*RTT-VT*VRZO*RTTO)*RDTVTO
      DC(IT+3)=DC(IT+3)+ACOEF*RV*
     1     (UW*DUOWDB4+UOW*DUWDB4)
      DC(IT+4)=DC(IT+4)+ACOEF*RV*
     1     (UW*DUOWDB5+UOW*DUWDB5)
      DC(IT+5)=DC(IT+5)+ACOEF*RV*
     1     (UW*DUOWDB6+UOW*DUWDB6)
      DC(IT+6)=DC(IT+6)+ACOEF*RUW*(VTO*DEXP(Z)-VT*DEXP(ZO))*RDTVTO
      IF(NOLAM(L,J))  GO TO 5300
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 5300
      DC(IT-2)=DC(IT-2)+
     1      ACOEF*RUW*A12*(VTO*DLDC1-VT*DLDC10)*RDTVTO
      DC(IT-3)=DC(IT-3)+
     1      ACOEF*RUW*A13*(VTO*DLDC1-VT*DLDC10)*RDTVTO
      IF(TAU.LE.ONE)  GO TO 5300
      DC(IT-1)=DC(IT-1)+
     1      ACOEF*RUW*A12*(VTO*DLDC2-VT*DLDC20)*RDTVTO
      DC(IT-3)=DC(IT-3)+
     1      ACOEF*RUW*A14*(VTO*DLDC2-VT*DLDC20)*RDTVTO
 5300 CONTINUE
      GO TO 8900
C
---------------------------------------------------------------
C     1 DV
C     - --  =  1/(B4 + B5*T + B6*P)  =  1/(BULK MODULUS)
C     V DP
C
C          WHERE TEMPERATURE IS CONSTANT.
```

```
C     SETTING "IGO(J)=19" FITS THE FUNCTION FOR THE BULK MODULUS.
C
C     FOR DATA MEASURED AT PREF OR LESS, "P" IS SET TO 0.0D0.
C
----------------------------------------------------------------------
 6000 CONTINUE
      IF(IGO(J).EQ.19)  GO TO 6100
      KBM=B4+B5*T
      IF(P.LE.PREF)  P=0.D0
      Y=Y+ACOEF/(KBM+B6*P)
      IF(JDFLAG.NE.0)  GO TO 8900
C     DC(IT)=DC(IT)+ZERO
C     DC(IT+1)=DC(IT+1)+ZERO
C     DC(IT+2)=DC(IT+2)+ZERO
      DC(IT+3)=DC(IT+3)-ACOEF/(KBM+B6*P)**2
      DC(IT+4)=DC(IT+4)-ACOEF*T/(KBM+B6*P)**2
      DC(IT+5)=DC(IT+5)-ACOEF*P/(KBM+B6*P)**2
C     DC(IT+6)=DC(IT+6)+ZERO
      GO TO 8900
 6100 CONTINUE
      IF(P.LE.PREF)  P=0.D0
      Y=Y+ACOEF*(B4+B5*T+B6*P)
      IF(JDFLAG.NE.0)  GO TO 8900
C     DC(IT)=DC(IT)+ZERO
C     DC(IT+1)=DC(IT+1)+ZERO
C     DC(IT+2)=DC(IT+2)+ZERO
      DC(IT+3)=DC(IT+3)+ACOEF
      DC(IT+4)=DC(IT+4)+ACOEF*T
      DC(IT+5)=DC(IT+5)+ACOEF*P
C     DC(IT+6)=DC(IT+6)+ZERO
      GO TO 8900
C
----------------------------------------------------------------------
C     YC = [V(T,P)-V(T,PO)]/[V(T,PO)*DP]
C
C        WHERE "DP" = P-PO.
C
C      THE SAME PHASE IS EVALUATED BOTH AT (T,P) AND (T,PO).  IF
"IGO(J)"
C        = 20, DP IS SET EQUAL TO 1.D0.
C
----------------------------------------------------------------------
 7000 CONTINUE
      IF(P.LE.PREF)  P=0.D0
      IF(PO.LE.PREF)  PO=0.D0
      KBM=B4+B5*T
      U=ONE+B6*P/KBM
      UO=ONE+B6*PO/KBM
      W=-ONE/B6
      UW=U**W
      UOW=UO**(-W)
      DP=P-PO
      IF(IGO(J).EQ.20)  DP=ONE
      Y=Y+ACOEF*(UW*UOW-ONE)/DP
```

```
      IF(JDFLAG.NE.0)  GO TO 8900
      WUWL1=W*U**(W-ONE)
      WUOWL1=-W*UO**(-(W+ONE))
      DUDB4=-B6*P/KBM**2
      DUDB5=DUDB4*T
      DUDB6=P/KBM
      DUODB4=-B6*PO/KBM**2
      DUODB5=DUODB4*T
      DUODB6=PO/KBM
      DWDB6=B6**(-2)
      DUWDB4=WUWL1*DUDB4
      DUWDB5=WUWL1*DUDB5
      DUWDB6=WUWL1*DUDB6+UW*DLOG(U)*DWDB6
      DUOWDB4=WUOWL1*DUODB4
      DUOWDB5=WUOWL1*DUODB5
      DUOWDB6=WUOWL1*DUODB6-UOW*DLOG(UO)*DWDB6
C     DC(IT)=DC(IT)+ZERO
C     DC(IT+1)=DC(IT+1)+ZERO
C     DC(IT+2)=DC(IT+2)+ZERO
      DC(IT+3)=DC(IT+3)+ACOEF*
     1     (UOW*DUWDB4+UW*DUOWDB4)
      DC(IT+4)=DC(IT+4)+ACOEF*
     1     (UOW*DUWDB5+UW*DUOWDB5)
      DC(IT+5)=DC(IT+5)+ACOEF*
     1     (UOW*DUWDB6+UW*DUOWDB6)
C     DC(IT+6)=DC(IT+6)+ZERO
      GO TO 8900
C
------------------------------------------------------------------
C
C     G(T,P) = G(T,PO) + INTEGRAL { V DP } FROM PO TO P.
C
C
------------------------------------------------------------------
 8000 CONTINUE
      Z=B1*T+B2*T*T/TWO-DEBT*B3*RTT
      VRZ=VR*DEXP(Z)
      VT=VRZ
      IF(NOLAM(L,J)) GO TO 8100
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 8100
      TAU=T/TC
      CALL LYDRIV(T,3,INDEX,JL,JH,JT)
      VT=VT+A12*A13*DLYDC(1)
      IF(TAU.LE.ONE)  GO TO 8100
      VT=VT+A12*A14*DLYDC(2)
 8100 CONTINUE
      KBM=B4+B5*T
      U=ONE+B6*P/KBM
      W=-ONE/B6
      UO=ONE+B6*PO/KBM
      UWP1=U**(W+ONE)
      UOWP1=UO**(W+ONE)
      INTVDP=KBM*(UWP1-UOWP1)/(B6-ONE)
      Y=Y+0.1D0*ACOEF*VT*INTVDP
```

```
      IF(JDFLAG.NE.0)  GO TO 8900
      DUDB4=-B6*P/KBM**2
      DUDB5=DUDB4*T
      DUDB6=P/KBM
      DWDB6=B6**(-2)
      WP1UW=(W+ONE)*U**W
      DUWDB4=WP1UW*DUDB4
      DUWDB5=WP1UW*DUDB5
      DUWDB6=WP1UW*DUDB6+UWP1*DLOG(U)*DWDB6
      DUODB4=-B6*PO/KBM**2
      DUODB5=DUODB4*T
      DUODB6=PO/KBM
      WP1UOW=(W+ONE)*UO**W
      DUOWDB4=WP1UOW*DUODB4
      DUOWDB5=WP1UOW*DUODB5
      DUOWDB6=WP1UOW*DUODB6+UOWP1*DLOG(UO)*DWDB6
      DC(IT)=DC(IT)+0.1D0*ACOEF*INTVDP*VRZ*T
      DC(IT+1)=DC(IT+1)+0.1D0*ACOEF*INTVDP*VRZ*T*T/TWO
      DC(IT+2)=DC(IT+2)-0.1D0*ACOEF*INTVDP*DEBT*VRZ*RTT
      DC(IT+3)=DC(IT+3)+0.1D0*ACOEF*VT*
     1     (KBM*(DUWDB4-DUOWDB4)+UWP1-UOWP1)/(B6-ONE)
      DC(IT+4)=DC(IT+4)+0.1D0*ACOEF*VT*
     1     (KBM*(DUWDB5-DUOWDB5)+(UWP1-UOWP1)*T)/(B6-ONE)
      DC(IT+5)=DC(IT+5)+0.1D0*VT*
     1   KBM*((DUWDB6-DUOWDB6)/(B6-ONE)-(UWP1-UOWP1)/(B6-ONE)**2)

      DC(IT+6)=DC(IT+6)+0.1D0*ACOEF*INTVDP*DEXP(Z)
      IF(NOLAM(L,J))  GO TO 8200
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 8200
      DC(IT-2)=DC(IT-2)+0.1D0*ACOEF*A12*DLYDC(1)*INTVDP
      DC(IT-3)=DC(IT-3)+0.1D0*ACOEF*A13*DLYDC(1)*INTVDP
      IF(TAU.LE.ONE)  GO TO 8200
      DC(IT-1)=DC(IT-1)+0.1D0*ACOEF*A12*DLYDC(2)*INTVDP
      DC(IT-3)=DC(IT-3)+0.1D0*ACOEF*A14*DLYDC(2)*INTVDP
 8200 CONTINUE
 8900 CONTINUE
      RETURN
C
----------------------------------------------------------------------
C    THE FOLLOWING ROUTINE WILL CALCULATE THE VOLUME RATIO AS DOES

C        THE  SECTION  ABOVE  BEGINNING  AT  STATEMENT  3000.   THE
DIFFERENCE
C    HERE IS THAT THE PHASE AT P AND T NEED NOT BE THE SAME AS THE

C    PHASE AT PO AND TO.  THE ROUTINE AT STATEMENT 3000 IS INVOKED
WHEN
C     THE NUMBER OF PHASES SPECIFIED IS NOT EQUAL TO 2.  THE
C     ROUTINE HERE IS INVOKED WHEN THE NUMBER OF PHASES IS 2.
C
C    THE STOICHIOMETRIC COEFFICIENT FOR THE PHASE AT THE REFERENCE

C     TEMPERATURE AND PRESSURE SHOULD BE NEGATIVE.  THIS WILL BE
TAKEN
```

```
C     AS THE PHASE IN THE DENOMINATOR OF THE VOLUME RATIO.
C
C
C     FOR DATA MEASURED AT PREF OR LESS, "P" IS SET TO 0.0D0.  THE
SAME
C        ALSO HOLDS FOR "PO".
C
---------------------------------------------------------------------
 9000 CONTINUE
      DO 9100 LL=1,2
      IF(COEF(LL,J).EQ.ZERO)  GO TO 9991
      IF(COEF(LL,J).LT.ZERO)  LO=LL
      IF(COEF(LL,J).GT.ZERO)  L=LL
 9100 CONTINUE
      IPH=IPHASE(L,J)
      IPHO=IPHASE(LO,J)
      INDEX=1+NPARM*(IPH-1)
      IT=INDEX+NCPARM+NMPARM
      INDEXO=1+NPARM*(IPHO-1)
      ITO=INDEXO+NCPARM+NMPARM
      B1=PC(IT)
      B2=PC(IT+1)
      B3=PC(IT+2)
      B4=PC(IT+3)
      B5=PC(IT+4)
      B6=PC(IT+5)
      VR=PC(IT+6)
      DEBT=PC(IT+7)
      A12=PC(IT-3)
      A13=PC(IT-2)
      A14=PC(IT-1)
      BO1=PC(ITO)
      BO2=PC(ITO+1)
      BO3=PC(ITO+2)
      BO4=PC(ITO+3)
      BO5=PC(ITO+4)
      BO6=PC(ITO+5)
      VRO=PC(ITO+6)
      DEBTO=PC(ITO+7)
      AO12=PC(ITO-3)
      AO13=PC(ITO-2)
      AO14=PC(ITO-1)
      ACACO=DABS(COEF(L,J)/COEF(LO,J))
      RTT=DEXP(-T/DEBT)
      Z=B1*T+B2*T*T/TWO-DEBT*B3*RTT
      VRZ=VR*DEXP(Z)
      VT=VRZ
      IF(NOLAM(L,J))  GO TO 9200
      IF(.NOT.LAMBDA(IPH))  GO TO 9200
      JL=PC(IT+8)
      JH=PC(IT+9)
      JT=PC(IT+10)
      TC=PC(IT-4)*(0.1d0*PC(IT-3)*(P-PREF)+ONE)
      PT=P
```

```
      TAU=T/TC
      CALL LYDRIV(T,3,INDEX,JL,JH,JT)
      VT=VT+A12*A13*DLYDC(1)
      DLDC1=DLYDC(1)
      IF(TAU.LE.ONE)  GO TO 9200
      VT=VT+A12*A14*DLYDC(2)
      DLDC2=DLYDC(2)
9200  CONTINUE
      KBM=B4+B5*T
      U=ONE+B6*P/KBM
      W=-ONE/B6
      UW=U**W
      V=VT*UW
      RTTO=DEXP(-TO/DEBTO)
      ZO=BO1*TO+BO2*TO*TO/TWO-DEBTO*BO3*RTTO
      VRZO=VRO*DEXP(ZO)
      VTO=VRZO
      IF(NOLAM(LO,J))  GO TO 9300
      IF(.NOT.LAMBDA(IPHO))  GO TO 9300
      JL=PC(ITO+8)
      JH=PC(ITO+9)
      JT=PC(ITO+10)
      TCO=PC(ITO-4)*(0.1D0*PC(ITO-3)*(PO-PREF)+ONE)
      PT=PO
      TAUO=TO/TCO
      CALL LYDRIV(TO,3,INDEXO,JL,JH,JT)
      VTO=VTO+AO12*AO13*DLYDC(1)
      DLDC1O=DLYDC(1)
      IF(TAUO.LE.ONE)  GO TO 9300
      VTO=VTO+AO12*AO14*DLYDC(2)
      DLDC2O=DLYDC(2)
9300  CONTINUE
      IF(PO.LE.PREF)  PO=0.D0
      KBMO=BO4+BO5*TO
      UO=ONE+BO6*PO/(KBMO)
      WO=-ONE/BO6
      UOW=UO**WO
      VO=VTO*UOW
      Y=ACACO*V/VO
      IF(JDFLAG.NE.0)  GO TO 9500
      RVO=ONE/VO
      RVOSQ=-ONE/(VO*VO)
      DUDB4=-B6*P/KBM**2
      DUDB5=DUDB4*T
      DUDB6=P/KBM
      DWDB6=B6**(-2)
      WUWL1=W*U**(W-ONE)
      DUWDB4=WUWL1*DUDB4
      DUWDB5=WUWL1*DUDB5
      DUWDB6=WUWL1*DUDB6+UW*DLOG(U)*DWDB6
      DC(IT)=DC(IT)+ACACO*UW*VRZ*T*RVO
      DC(IT+1)=DC(IT+1)+ACACO*UW*VRZ*T*T*RVO/TWO
      DC(IT+2)=DC(IT+2)-ACACO*UW*VRZ*DEBT*RTT*RVO
      DC(IT+3)=DC(IT+3)+ACACO*VT*RVO*DUWDB4
```

```
      DC(IT+4)=DC(IT+4)+ACACO*VT*RVO*DUWDB5
      DC(IT+5)=DC(IT+5)+ACACO*VT*RVO*DUWDB6
      DC(IT+6)=DC(IT+6)+ACACO*UW*DEXP(Z)*RVO
      IF(NOLAM(L,J))  GO TO 9400
      IF(.NOT.LAMBDA(IPH))  GO TO 9400
      DC(IT-2)=DC(IT-2)+ACACO*UW*A12*DLDC1*RVO
      DC(IT-3)=DC(IT-3)+ACACO*UW*A13*DLDC1*RVO
      IF(TAU.LE.ONE)  GO TO 9400
      DC(IT-1)=DC(IT-1)+ACACO*UW*A12*DLDC2*RVO
      DC(IT-3)=DC(IT-3)+ACACO*UW*A14*DLDC2*RVO
 9400 CONTINUE
      DUODB4=-BO6*PO/KBMO**2
      DUODB5=DUODB4*TO
      DUODB6=PO/KBMO
      DWODB6=BO6**(-2)
      WUOWL1=WO*UO**(WO-ONE)
      DUOWDB4=WUOWL1*DUODB4
      DUOWDB5=WUOWL1*DUODB5
      DUOWDB6=WUOWL1*DUODB6+UOW*DLOG(UO)*DWODB6
      DC(ITO)=DC(ITO)-ACACO*V*UOW*VRZO*T*RVOSQ
      DC(ITO+1)=DC(ITO+1)-ACACO*V*UOW*VRZO*T*TO*RVOSQ/TWO
      DC(ITO+2)=DC(ITO+2)+ACACO*V*UOW*VRZO*DEBT*RTTO*RVOSQ
      DC(ITO+3)=DC(ITO+3)-ACACO*V*VTO*DUOWDB4*RVOSQ
      DC(ITO+4)=DC(ITO+4)-ACACO*V*VTO*DUOWDB5*RVOSQ
      DC(ITO+5)=DC(ITO+5)-ACACO*V*VTO*DUOWDB6*RVOSQ
      DC(ITO+6)=DC(ITO+6)-ACACO*V*UOW*DEXP(ZO)*RVOSQ
      IF(NOLAM(LO,J))  GO TO 9500
      IF(.NOT.LAMBDA(IPHO))  GO TO 9500
      DC(ITO-2)=DC(ITO-2)-ACACO*V*UOW*AO12*DLDC10*RVOSQ
      DC(ITO-3)=DC(ITO-3)-ACACO*V*UOW*AO13*DLDC10*RVOSQ
      IF(TAUO.LE.ONE)  GO TO 9500
      DC(ITO-1)=DC(ITO-1)-ACACO*V*UOW*AO12*DLDC20*RVOSQ
      DC(ITO-3)=DC(ITO-3)-ACACO*V*UOW*AO14*DLDC20*RVOSQ
 9500 CONTINUE
      RETURN
 9990 CONTINUE
      WRITE (60,60)IGO(J)
      STOP
 9991 CONTINUE
      WRITE (60,61)J
      STOP
C
----------------------------------------------------------------------
   60 FORMAT ('0*****  THE VOLUME FUNCTION FOR IGO(J) = ',I3,' IS
NOT PR
     1OGRAMMED.   *****')
   61 FORMAT ('0*****    A COEFFICIENT IN YOUR DATA SET NUMBER
',I4,' IS
     1ZERO.    ****')
C
----------------------------------------------------------------------
      END
      SUBROUTINE MISCFN(YC,I,J,JDFLAG)
C
```

```
-----------------------------------------------------------------
C
C     "MISCFN" WILL CALCULATE THE FOLLOWING FUNCTIONS:
C          IGO(J)= 9 IMPLIES CV(T,1), HEAT CAPACITY AT CONSTANT
VOLUME.
C                   IGO(J)=23  IMPLIES  KAPPA-S(T,1),  ISENTROPIC
COMPRESSIBILITY.
C          IGO(J)=24 IMPLIES BMS(T,1), ISENTROPIC BULK MODULUS.
C          IGO(J)=25 IMPLIES GRUNEISEN CONSTANT, GAMMA.
C     LAST REVISED 1 DEC 1988 BY HAAS.
C
-----------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL*1 LAMBDA,NOLAM,UNDAMP
      REAL*8 KAPPAS,KAPPAT
C
-----------------------------------------------------------------
C
C       PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C         DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C         MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------
      DIMENSION DCV(NPARM),DCA(NPARM),DCK(NPARM),DCBMT(NPARM),
     1          DCCP(NPARM)
      DIMENSION COEF(IP4,IP3),TINV(IP4,IP3,IP10),NPHASE(IP3),
                1
IKOUNT(IP3),IGO(IP3),ISTATE(IP4,IP3),INSTAT(IP4,IP3),
     2         INVPH(IP4,IP3,IP11),INVSC(IP4,IP3),ISPECL(IP4,IP3),
     3          IPHASE(IP4,IP3),NINVER(IP4,IP3)
                                 DIMENSION
X(NX,IP2),PC(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1          ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION DYDC(NCPARM),DHDC(NCPARM),DGDC(NCPARM),DLYDC(2),
     1          DLHDC(2),DLGDC(2)
      DIMENSION LAMBDA(IP1),NOLAM(IP4,IP3)
      COMMON /EARTH/ COEF,TINV,NPHASE,IKOUNT,IGO,ISTATE,INSTAT,
     1               INVPH,INVSC,ISPECL,IPHASE,NINVER,NSETS,LISTP
      COMMON /AIR/ X,PC,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1             ISING,ISTOP,IL,JDF,ION
                             COMMON          /WATER/
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1               STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /SPACE/ DYDC,DHDC,DGDC,DLYDC,DLHDC,DLGDC,SC,TO,PT
      COMMON /AETHER/ LAMBDA,NOLAM,UNDAMP
```

```
C
-----------------------------------------------------------------
C     INITIALIZE THE CONSTANTS.
C
-----------------------------------------------------------------
      YC=0.D0
      DO 100 N=1,NP
      DC(N)=ZERO
  100 CONTINUE
      YC=ZERO
      T=X(1,I)
      P=X(3,I)
      IF(P.NE.ZERO)  GO TO 200
      P=PREF
      X(3,I)=PREF
  200 CONTINUE
      LAST=NPHASE(J)
      PT=PREF
C
-----------------------------------------------------------------
C     IF IGO(J)= 9, " 9-21" =<1 AND IMPLIES CV DATA.
C             =23, "23-21" = 2 AND IMPLIES KAPPA-S DATA.
C             =24, "24-21" = 3 AND IMPLIES BMS DATA.
C             =25, "25-21" = 4 AND IMPLIES GRUNEISEN GAMMA DATA.
C
-----------------------------------------------------------------
      IGOES=IGO(J)-21
      IF(IGOES.LE.1)  IGOES=1
C
-----------------------------------------------------------------
C      INITIALIZE CONSTANTS AND CALCULATE THE PROPERTIES OF EACH
PHASE.
C
-----------------------------------------------------------------
      DO 8000 L=1,LAST
      ACOEF=COEF(L,J)
      INDEX=1+NPARM*(IPHASE(L,J)-1)
      IT=NCPARM+NMPARM
      B1=PC(INDEX+IT)
      B2=PC(INDEX+IT+1)
      B3=PC(INDEX+IT+2)
      B4=PC(INDEX+IT+3)
      B5=PC(INDEX+IT+4)
      B6=PC(INDEX+IT+5)
      VR=PC(INDEX+IT+6)
      DEBT=PC(INDEX+IT+7)
      RTT=DEXP(-T/DEBT)
      IF(NOLAM(L,J))  GO TO 300
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 300
      A12=PC(INDEX+IT-3)
      TC=PC(INDEX+IT-4)*(0.1d0*PC(INDEX+IT-3)*(P-PREF)+ONE)
      PT=P
      A13=PC(INDEX+IT-2)
      A14=PC(INDEX+IT-1)
```

```
      TAU=T/TC
      JL=PC(INDEX+IT+8)
      JH=PC(INDEX+IT+9)
      JT=PC(INDEX+IT+10)
  300 CONTINUE
      DO 400 K=1,NPARM
      DCV(K)=ZERO
      DCA(K)=ZERO
      DCK(K)=ZERO
      DCCP(K)=ZERO
      DCBMT(K)=ZERO
  400 CONTINUE
C
------------------------------------------------------------------
C     CALCULATE THE MOLAR VOLUME, V, AND DERIVATIVES.
C
------------------------------------------------------------------
 1000 CONTINUE
      IF(P.LE.PREF)  P=ZERO
      BMTO=B4+B5*T
      U=ONE+B6*P/BMTO
      W=-ONE/B6
      UW=U**W
      Z=B1*T+B2*T*T/TWO-DEBT*B3*RTT
      VRZ=VR*DEXP(Z)
      VT=VRZ
      IF(NOLAM(L,J))  GO TO 1100
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 1100
      CALL LYDRIV(T,3,INDEX,JL,JH,JT)
      DLDC10=DLYDC(1)
      DLDC20=DLYDC(2)
      VT=VT+A12*A13*DLDC10
      DCV(IT-1)=DCV(IT-1)+ACOEF*UW*A12*DLDC10
      DCV(IT-2)=DCV(IT-2)+ACOEF*UW*A13*DLDC10
      IF(TAU.LE.ONE)  GO TO 1100
      VT=VT+A12*A14*DLDC20
      DCV(IT)=DCV(IT)+ACOEF*UW*A12*DLDC20
      DCV(IT-2)=DCV(IT-2)+ACOEF*UW*A14*DLDC20
 1100 CONTINUE
      V=ACOEF*VT*UW
      IF(JDFLAG.NE.0)  GO TO 2000
      DUDB4=-B6*P/BMTO**2
      DUDB5=DUDB4*T
      DUDB6=P/BMTO
      DWDB6=B6**(-2)
      WUWL1=W*U**(W-ONE)
      DCV(IT+1)=DCV(IT+1)+ACOEF*UW*VRZ*T
      DCV(IT+2)=DCV(IT+2)+ACOEF*UW*VRZ*T*T/TWO
      DCV(IT+3)=DCV(IT+3)-ACOEF*UW*VRZ*DEBT*RTT
      DCV(IT+4)=DCV(IT+4)+ACOEF*VT*WUWL1*DUDB4
      DCV(IT+5)=DCV(IT+5)+ACOEF*VT*WUWL1*DUDB5
      DCV(IT+6)=DCV(IT+6)+ACOEF*VT*
     1     (WUWL1*DUDB6+UW*DLOG(U)*DWDB6)
      DCV(IT+7)=DCV(IT+7)+ACOEF*UW*DEXP(Z)
```

```
C
-----------------------------------------------------------------
C          CALCULATE  THE  EXPANSIVITY  COEFFICIENT,  ALPHA,  AND
DERIVATIVES.
C
-----------------------------------------------------------------
 2000 CONTINUE
      ALPH=B1+B2*T+B3*RTT
      DVMDT=ZERO
      IF(NOLAM(L,J))  GO TO 2200
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 2200
      CALL LYDRIV(T,1,INDEX,JL,JH,JT)
      DLDC1=DLYDC(1)
      DLDC2=DLYDC(2)
      IF(TAU.GT.ONE)  GO TO 2100
      DVMDT=DVMDT+A12*A13*DLDC1
      GO TO 2200
 2100 CONTINUE
      DVMDT=DVMDT+A12*A14*DLDC2
 2200 CONTINUE
      F1=1.D0/(BMTO+B6*P)
      F2=1.D0/BMTO
      ALPHA=ACOEF*(B5*P*F1*F2+(ALPH*VRZ+DVMDT)/VT)
      IF(JDFLAG.NE.0)  GO TO 2300
      DVTDT=VRZ*ALPH+DVMDT
      DCA(IT+1)=DCA(IT+1)+ACOEF*VRZ*(1.D0+ALPH*T-DVTDT*T/VT)/VT

DCA(IT+2)=DCA(IT+2)+VRZ*T*(1.D0+ALPH*T/2.D0-DVTDT*T/(2.D0*VT))/VT
      DCA(IT+3)=DCA(IT+3)+VRZ*RTT*(1.D0-ALPH*DEBT+DVTDT*DEBT/VT)/VT
      DCA(IT+4)=DCA(IT+4)-B5*P*F1*F2*(F2+F1)
      DCA(IT+5)=DCA(IT+5)+F1*F2*P*(1.D0-B5*F1*T-B5*F2*T)
      DCA(IT+6)=DCA(IT+6)-B5*P*P*F1*F2*(F2+F1)
      DCA(IT+7)=DCA(IT+7)+DEXP(Z)*(ALPH-DVTDT/VT)/VT
      IF(NOLAM(L,J))  GO TO 2300
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 2300
      DCA(IT-1)=DCA(IT-1)+
     1           ACOEF*A12*(DLDC1-DVMDT*DLDC10/VT)/VT
      DCA(IT-2)=DCA(IT-2)+
     1           ACOEF*A13*(DLDC1-DVMDT*DLDC10/VT)/VT
      IF(TAU.LE.ONE)  GO TO 2300
      DCA(IT)=DCA(IT)+
     1           ACOEF*A12*(DLDC2-DVMDT*DLDC20/VT)/VT
      DCA(IT-2)=DCA(IT-2)+
     1           ACOEF*A14*(DLDC2-DVMDT*DLDC20/VT)/VT
 2300 CONTINUE
C
-----------------------------------------------------------------
C     CALCULATE THE ISOTHERMAL COMPRESSIBILITY, KAPPA(T), OR THE
C        ISOTHERMAL BULK MODULUS, BMT(T), AND THE DERIVATIVES.
C
-----------------------------------------------------------------
 3000 CONTINUE
      IF(IGOES.EQ.1)  GO TO 3100
      KAPPAT=ACOEF/(BMTO+B6*P)
```

```
      IF(JDFLAG.NE.0)  GO TO 3200
C     DCK(IT+1)=DCK(IT+1)+ZERO
C     DCK(IT+2)=DCK(IT+2)+ZERO
C     DCK(IT+3)=DCK(IT+3)+ZERO
      DCK(IT+4)=DCK(IT+4)-ACOEF/(BMTO+B6*P)**2
      DCK(IT+5)=DCK(IT+5)-ACOEF*T/(BMTO+B6*P)**2
      DCK(IT+6)=DCK(IT+6)-ACOEF*P/(BMTO+B6*P)**2
C     DCK(IT+7)=DCK(IT+7)+ZERO
      GO TO 3200
 3100 CONTINUE
      BMT=BMTO+B6*P
      IF(JDFLAG.NE.0)  GO TO 3200
C     DCBMT(IT+1)=DCBMT(IT+1)+ZERO
C     DCBMT(IT+2)=DCBMT(IT+2)+ZERO
C     DCBMT(IT+3)=DCBMT(IT+3)+ZERO
      DCBMT(IT+4)=DCBMT(IT+4)+ONE
      DCBMT(IT+5)=DCBMT(IT+5)+T
      DCBMT(IT+6)=DCBMT(IT+6)+P
C     DCBMT(IT+7)=DCBMT(IT+7)+ZERO
 3200 CONTINUE
C
------------------------------------------------------------------
C     CALCULATE THE MOLAR HEAT CAPACITY, CP, AND DERIVATIVES.
C
------------------------------------------------------------------
 4000 CONTINUE
      CP=ZERO
      CALL YDERIV(T,1)
      DO 4100 K=1,NCPARM
      DCCP(K)=DCCP(K)+ACOEF*DYDC(K)
      CP=CP+ACOEF*DYDC(K)*PC(INDEX+K-1)
 4100 CONTINUE
      IF(NOLAM(L,J))  GO TO 4300
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 4300
      IF (T.GT.TC)  GO TO 4200
      DCCP(IT-2)=DCCP(IT-2)+ACOEF*DLDC1
      CP=CP+ACOEF*DLDC1*PC(INDEX+IT-2)
      GO TO 4300
 4200 CONTINUE
      DCCP(IT-1)=DCCP(IT-1)+ACOEF*DLDC2
      CP=CP+ACOEF*DLDC2*PC(INDEX+IT-1)
 4300 CONTINUE
      GO TO (5000,6000,7000,7000),IGOES
C
------------------------------------------------------------------
C     CALCULATE CV, THE HEAT CAPACITY AT CONSTANT VOLUME.
C
C     CV = CP - 0.1 * T * ALPHA**2 * V * BMT
C
C
------------------------------------------------------------------
 5000 CONTINUE
      CV=CP-0.1D0*T*ALPHA**2*V*BMT
      YC=YC+CV
```

```
      IF(JDFLAG.NE.0)  GO TO 9000
      DO 5100 K=1,NCPARM
      DC(INDEX+K-1)=DC(INDEX+K-1)+DCCP(K)
 5100 CONTINUE
      K1=NCPARM+NMPARM+1
      K2=NCPARM+NMPARM+NVPARM-1
      DO 5200 K=K1,K2
      DC(INDEX+K-1)=DC(INDEX+K-1)-0.1D0*T*
     1     (ALPHA**2*V*DCBMT(K)
     1      +ALPHA**2*BMT*DCV(K)
     1      +V*T*2.D0*ALPHA*DCA(K))
 5200 CONTINUE
      IF(NOLAM(L,J))  GO TO 9000
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 9000
      K1=NCPARM+2
      K2=NCPARM+NMPARM
      DO 5300 K=K1,K2
      DC(INDEX+K-1)=DC(INDEX+K-1)+DCCP(K)-0.1D0*T*
     1     (ALPHA**2*V*DCBMT(K)
     1      +ALPHA**2*BMT*DCV(K)
     1      +V*T*2.D0*ALPHA*DCA(K))
 5300 CONTINUE
      GO TO 9000
C
-----------------------------------------------------------------
C     CALCULATED KAPPA(S), THE ISENTROPIC COMPRESSIBILITY.
C
C                                                0.1 * (ALPHA**2) * V
* T
C                  KAPPA(ISENTROPIC)    =    KAPPA(ISOTHERMAL)    -
------------------------
C                                                            Cp
C
C
-----------------------------------------------------------------
 6000 CONTINUE
      KAPPAS=KAPPAT-0.1D0*ALPHA**2*V*T/CP
      YC=YC+KAPPAS
      IF(JDFLAG.NE.0)  GO TO 9000
      DO 6100 K=1,NCPARM
      DC(INDEX+K-1)=DC(INDEX+K-1)+0.1D0*T*ALPHA**2*V*DCCP(K)/CP**2
 6100 CONTINUE
      K1=NCPARM+NMPARM+1
      K2=NCPARM+NMPARM+NVPARM-1
      DO 6200 K=K1,K2
      DC(INDEX+K-1)=DC(INDEX+K-1)+DCK(K)
     1     -0.1D0*T*ALPHA*(ALPHA*DCV(K)+TWO*V*DCA(K))/CP
 6200 CONTINUE
      IF(NOLAM(L,J))  GO TO 9000
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 9000
      K1=NCPARM+2
      K2=NCPARM+NMPARM
      DO 6300 K=K1,K2
      DC(INDEX+K-1)=DC(INDEX+K-1)+DCK(K)
```

```
     1     -0.1D0*T*(ALPHA**2*DCV(K)/CP+TWO*ALPHA*V*DCA(K)/CP
     2         -ALPHA**2*V*DCCP(K)/CP**2)
 6300 CONTINUE
      GO TO 9000
C
-----------------------------------------------------------------
C     CALCULATE THE ISENTROPIC BULK MODULUS, BMS.
C
C             1            CP
C     BMS = -- = ---------------------
C           KS   KT*CP-0.1*ALPHA**2*V*T
C
C
-----------------------------------------------------------------
 7000 CONTINUE
      DENOM2=-0.1D0*T*ALPHA*ALPHA*V
      DENOM=KAPPAT*CP+DENOM2
      BMS=CP/DENOM
      YC=YC+BMS
      IF(JDFLAG.NE.0)  GO TO 9000
      RDENSQ=1.D0/(DENOM*DENOM)
      DO 7100 K=1,NCPARM
      DC(INDEX+K-1)=DC(INDEX+K-1)
     1     +(DENOM*DCCP(K)-CP*KAPPAT*DCCP(K))*RDENSQ
 7100 CONTINUE
      K1=NCPARM+NMPARM+1
      K2=NCPARM+NMPARM+NVPARM-1
      DO 7200 K=K1,K2
      DC(INDEX+K-1)=DC(INDEX+K-1)
                                                    1
-CP*(CP*DC(K)-0.1D0*T*ALPHA*(ALPHA*DCV(K)+2.D0*V*DCA(K)))
     1     *RDENSQ
 7200 CONTINUE
      IF(NOLAM(L,J))  GO TO 9000
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 9000
      K1=NCPARM+2
      K2=NCPARM+NMPARM
      DO 7300 K=K1,K2
      DC(INDEX+K-1)=DC(INDEX+K-1)+(DENOM*DCCP(K)
     1     -CP*(KAPPAT*DCCP(K)+CP*DCK(K)
     1     -0.1D0*T*ALPHA*(ALPHA*DCV(K)+2.D0*V*DCA(K))))*RDENSQ
 7300 CONTINUE
      IF(IGOES.NE.4)  GO TO 9000
C
-----------------------------------------------------------------
C     CALCULATE GAMMA, THE GRUENEISEN CONSTANT.
C
C             0.1 * ALPHA * BM-S * V
C     GAMMA = ---------------------
C                       CP
C
C
-----------------------------------------------------------------
 8000 CONTINUE
```

```
C
-----------------------------------------------------------------------
C     THE GRUENEISEN CONSTANT HAS NOT BEEN PROGRAMMED.  THE PRESENT
C          CODE CALCULATES THE GRUENEISEN CONSTANT BUT DOES NOT DO
THE
C          ADDITIONAL CALCULATIONS SO THAT THE GRUENEISEN CONSTANT
MAY BE
C         PART OF THE OPTIMIZED DATA.
C
-----------------------------------------------------------------------
      YC=0.1D0*ALPHA*BMS*V/CP
 9000 CONTINUE
      RETURN
      END
      SUBROUTINE TCFIT(YC,I,J)
C
-----------------------------------------------------------------------
C
C         "TCFIT"  IS  DESIGNED  TO  ALLOW  FITTING  OF  THE  CRITICAL
TEMPERATURES
C            FOR  LAMBDA  ANOMALIES  TO  A  1ST  ORDER  POLYNOMIAL  IN
PRESSURE:
C
C         Tc = Tc(@ PREF)*(0.1*A(12,i)*(P-PREF) + 1.D0)
C
C     LAST REVISED 1 DEC 1988 BY HAAS.
C
-----------------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
C
-----------------------------------------------------------------------
C
C        PARAMETERS  STATEMENTS.   THESE  HAVE  BEEN  ENTERED  IN  EACH
ROUTINE
C         IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C          DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C          MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C         ALSO.
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------------
      DIMENSION COEF(IP4,IP3),TINV(IP4,IP3,IP10),NPHASE(IP3),
               1
IKOUNT(IP3),IGO(IP3),ISTATE(IP4,IP3),INSTAT(IP4,IP3),
     2        INVPH(IP4,IP3,IP11),INVSC(IP4,IP3),ISPECL(IP4,IP3),
     3          IPHASE(IP4,IP3),NINVER(IP4,IP3)
                            D    I    M    E    N    S    I    O    N
X(NX,IP2),PC(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1          ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
```

```
      COMMON /EARTH/ COEF,TINV,NPHASE,IKOUNT,IGO,ISTATE,INSTAT,
     1               INVPH,INVSC,ISPECL,IPHASE,NINVER,NSETS,LISTP
      COMMON /AIR/ X,PC,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1             ISING,ISTOP,IL,JDF,ION
                    C   O   M   M   O   N       /   W   A   T   E   R   /
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1               STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
C
-------------------------------------------------------------------
C     INITIALIZE VARIABLES
C
-------------------------------------------------------------------
      P=X(3,I)
      IF(P.EQ.0.D0) P=PREF
      DP=P-PREF
      INDEX=1+NPARM*(IPHASE(1,J)-1)
      TCO=PC(INDEX+NCPARM)
      DTC=PC(INDEX+NCPARM+1)
      DO 1000 N=1,NPARM
      DC(N)=0.D0
 1000 CONTINUE
C
-------------------------------------------------------------------
C        CALCULATE  THE  CRITICAL  TEMPERATURE  AT  T  AND  P,  THE
DERIVATIVES,
C        AND RETURN.
C
-------------------------------------------------------------------
      YC=TCO*(0.1D0*DTC*DP+1.D0)
      DC(INDEX+10)=0.1D0*DTC*DP+1.D0
      DC(INDEX+11)=0.1D0*TCO*DP
      RETURN
      END
      SUBROUTINE DPDT(YC,I,J,JDFLAG)
C
-------------------------------------------------------------------
C
C    "DPDT" CALCULATES THE INITIAL SLOPE OF A P-T CURVE AT P=0.D0.
C       THE CALCULATING ALGORITHM IS AS FOLLOWS:
C
C
C       YC = DELTA(S)/DELTA(V)
C
C
C        WHERE DELTA(S) AND DELTA(V) ARE THE ENTROPY AND VOLUME
CHANGES
C       FOR THE CHEMICAL REACTION.
C
C     LAST REVISED MARCH, 1990 BY HAAS TO CORRECT AN ERROR IN THE
C       ENERGY-VOLUME CONVERSION FACTOR.
C
-------------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL*1 LAMBDA,NOLAM,UNDAMP
```

```
      REAL*8 KBM
C
---------------------------------------------------------------------
C
C       PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C         DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C         MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
---------------------------------------------------------------------
      DIMENSION VT(IP4),VP(IP4),DLYDC1(IP4),DLYDC2(IP4),INDEX(IP4),
               1
ITEM(IP4),TC(IP4),A12(IP4),A13(IP4),A14(IP4),TAU(IP4),
     2         ACOEF(IP4),B1(IP4),B2(IP4),B3(IP4),B4(IP4),B5(IP4),
     3         B6(IP4),VR(IP4),DEBT(IP4),Z(IP4),VRZ(IP4),RTT(IP4),
     4           WUWL1(IP4),KBM(IP4)
      DIMENSION COEF(IP4,IP3),TINV(IP4,IP3,IP10),NPHASE(IP3),
               1
IKOUNT(IP3),IGO(IP3),ISTATE(IP4,IP3),INSTAT(IP4,IP3),
     2         INVPH(IP4,IP3,IP11),INVSC(IP4,IP3),ISPECL(IP4,IP3),
     3           IPHASE(IP4,IP3),NINVER(IP4,IP3)
                           D  I  M  E  N  S  I  O  N
X(NX,IP2),PC(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1         ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION DYDC(NCPARM),DHDC(NCPARM),DGDC(NCPARM),DLYDC(2),
     1           DLHDC(2),DLGDC(2)
      DIMENSION LAMBDA(IP1),NOLAM(IP4,IP3)
      COMMON /EARTH/ COEF,TINV,NPHASE,IKOUNT,IGO,ISTATE,INSTAT,
     1               INVPH,INVSC,ISPECL,IPHASE,NINVER,NSETS,LISTP
      COMMON /AIR/ X,PC,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1             ISING,ISTOP,IL,JDF,ION
                 C  O  M  M  O  N     /  W  A  T  E  R  /
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1               STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /SPACE/ DYDC,DHDC,DGDC,DLYDC,DLHDC,DLGDC,SC,TO,PT
      COMMON /AETHER/ LAMBDA,NOLAM,UNDAMP
C
---------------------------------------------------------------------
C     ASSIGN INITIAL VALUES.
C
---------------------------------------------------------------------
      DV=0.D0
      T=X(1,I)
      IF(X(3,I).EQ.0.D0)  X(3,I)=PREF
      P=X(3,I)
      PT=P
```

```
C
-----------------------------------------------------------------
C     CALCULATE DELTA(S) FOR THE REACTION USING FNCALC.
C
-----------------------------------------------------------------
      DS=FNCALC(T,J,2)
C
-----------------------------------------------------------------
C     CALCULATE DELTA(V)
C
-----------------------------------------------------------------
      LAST=NPHASE(J)
      DO 2000 L=1,LAST
C
-----------------------------------------------------------------
C     INITIALIZE THE CONSTANTS FOR THE L-TH PHASE.
C
-----------------------------------------------------------------
      ACOEF(L)=COEF(L,J)
      INDEX(L)=1+NPARM*(IPHASE(L,J)-1)
      ITEM(L)=INDEX(L)+NCPARM+NMPARM
      B1(L)=PC(ITEM(L))
      B2(L)=PC(ITEM(L)+1)
      B3(L)=PC(ITEM(L)+2)
      VR(L)=PC(ITEM(L)+6)
      DEBT(L)=PC(ITEM(L)+7)
      RTT(L)=DEXP(-T/DEBT(L))
C                                                     *
-----------------------------------------------------------------
C*    THE CALCULATION OF VP(L) IS DELETED USING COMMENT CONTROLS
(C*  ).
C*       AT P=PREF (1 BAR) OR LESS, THE CHANGE DUE TO PRESSURE IS
NIL.
C                                                     *
-----------------------------------------------------------------
C*    B4(L)=PC(ITEM(L)+3)
C*    B5(L)=PC(ITEM(L)+4)
C*    B6(L)=PC(ITEM(L)+5)
C*    KBM(L)=B4(L)+B5(L)*T
C*    U=ONE+B6(L)*P/KBM(L)
C*    W=-ONE/B6(L)
C*    WUWL1(L)=W*U**(W-ONE)
C*    VP(L)=U**W
C
-----------------------------------------------------------------
C     CALCULATE VT(L).
C
C*    ALSO SET VP(L) = 1.D0 SO THAT AT SOME FUTURE TIME WHEN THE
SLOPE
C*       IS CALCULATED AT ELEVATED PRESSURES, MINIMAL ADJUSTMENTS
MUST
C*       BE MADE
C
-----------------------------------------------------------------
```

```
      VP(L)=1.D0
      Z(L)=B1(L)*T+B2(L)*T*T/TWO-DEBT(L)*B3(L)*RTT(L)
      VRZ(L)=VR(L)*DEXP(Z(L))
      VT(L)=VRZ(L)
      IF(NOLAM(L,J))  GO TO 1000
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 1000
      A12(L)=PC(ITEM(L)-3)
      TC(L)=PC(ITEM(L)-4)*(0.1D0*A12(L)*(P-PREF)+1.D0)
      A13(L)=PC(ITEM(L)-2)
      A14(L)=PC(ITEM(L)-1)
      TAU(L)=T/TC(L)
      IND=INDEX(L)
      JL=PC(ITEM(L)+8)
      JH=PC(ITEM(L)+9)
      JT=PC(ITEM(L)+10)
      CALL LYDRIV(T,3,IND,JL,JH,JT)
      DLYDC1(L)=DLYDC(1)
      DLYDC2(L)=DLYDC(2)
      VT(L)=VT(L)+A12(L)*A13(L)*DLYDC1(L)
      IF(TAU(L).LE.1.D0)  GO TO 1000
      VT(L)=VT(L)+A12(L)*A14(L)*DLYDC2(L)
 1000 CONTINUE
      DV=DV+ACOEF(L)*VT(L)*VP(L)
 2000 CONTINUE
C
----------------------------------------------------------------------
C     CALCULATE THE P-T SLOPE AND RETURN IF THIS IS THE LAST CYCLE.
C
----------------------------------------------------------------------
      YC=DS/(0.1D0*DV)
      IF(JDFLAG.NE.0)  GO TO 5000
      RDVSQ=1.D0/(DV*DV)
C
----------------------------------------------------------------------
C      CALCULATE THE FULL DERIVATIVE AND RETURN.
C
----------------------------------------------------------------------
      DO 4000 L=1,LAST
C
----------------------------------------------------------------------
C     CORRECT THE DERIVATIVES FOR DELTA(S) TO REFLECT THE DIVISOR
C        DELTA(V).
C
----------------------------------------------------------------------
      DO 3000 K=1,NCPARM
      DC(INDEX(L)+K-1)=DC(INDEX(L)+K-1)/(0.1D0*DV)
 3000 CONTINUE
C
----------------------------------------------------------------------
C     CALCULATE THE FULL DERIVATIVE FOR THE CONSTANTS IN THE VOLUME
C        EQUATION.
C
----------------------------------------------------------------------
```

```
DC(ITEM(L))=DC(ITEM(L))-DS*RDVSQ*ACOEF(L)*VP(L)*VRZ(L)*T/0.1D0

DC(ITEM(L)+1)=DC(ITEM(L)+1)-DS*RDVSQ*ACOEF(L)*VP(L)*VRZ(L)*T*T
     1              /(0.2D0)

DC(ITEM(L)+2)=DC(ITEM(L)+2)+DS*RDVSQ*ACOEF(L)*VP(L)*VRZ(L)*DEBT(L)
     1      *RTT(L)/0.1D0
C
-----------------------------------------------------------------
C     WITH VP(L) SET TO 1.D0, THE NEXT DERIVATIVE CALCULATIONS ARE
NOT
C        NEEDED.
C
-----------------------------------------------------------------
C     DC(ITEM(L)+3)=DC(ITEM(L)+3)
C                                                                 1
-DS*RDVSQ*ACOEF(L)*VT(L)*WUWL1(L)*(-B6(L)*P)/(0.1D0*KBM(L)**2
C     DC(ITEM(L)+4)=DC(ITEM(L)+4)
C                                                                 1
-DS*RDVSQ*ACOEF(L)*VT(L)*WUWL1(L)*(-B6(L)*T*P)/(0.1D0*KBM(L)**2)
C     DC(ITEM(L)+5)=DC(ITEM(L)+5)
C    1      -DS*RDVSQ*ACOEF(L)*VT(L)*(WUWL1(L)*P/KBM(L)
C    1      +VP(L)*DLOG(U)/(B6(L)*B6(L)))/0.1D0

DC(ITEM(L)+6)=DC(ITEM(L)+6)-DS*RDVSQ*ACOEF(L)*VP(L)*DEXP(Z(L))
     1      /0.1D0
C
-----------------------------------------------------------------
C        CALCULATE THE DERIVATIVES FOR THE LAMBDA-PART OF THE
FUNCTIONS.
C
-----------------------------------------------------------------
      IF(NOLAM(L,J))  GO TO 4000
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 4000
      IND1=ITEM(L)-2
      IND2=ITEM(L)-1
      IND6=ITEM(L)-3

DC(IND1)=DC(IND1)-DS*ACOEF(L)*VP(L)*A12(L)*DLYDC1(L)*RDVSQ/0.1D0

DC(IND6)=DC(IND6)-DS*ACOEF(L)*VP(L)*A13(L)*DLYDC1(L)*RDVSQ/0.1D0
      IF(TAU(L).LE.1.D0)  GO TO 4000

DC(IND2)=DC(IND2)-DS*ACOEF(L)*VP(L)*A12(L)*DLYDC2(L)*RDVSQ/0.1D0

DC(IND6)=DC(IND6)-DS*ACOEF(L)*VP(L)*A14(L)*DLYDC2(L)*RDVSQ/0.1D0
 4000 CONTINUE
C
-----------------------------------------------------------------
C     RETURN TO THE CALLING PROGRAM.
C
-----------------------------------------------------------------
 5000 CONTINUE
      RETURN
```

```
      END
      SUBROUTINE YDERIV(T,IGOES)
C
-----------------------------------------------------------------------
C
C                                             YDERIV
C     THIS VERSION WRITEN 3/09/72 BY HAAS.
C          LAST REVISED 8/05/72 BY HAAS.
C
C       REVISED  TO  ACCEPT  THE  CODATA  THERMAL  FUNCTION  BY  HAAS,
8/31/84.
C
C
-----------------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
C
-----------------------------------------------------------------------
C
C       PARAMETERS  STATEMENTS.   THESE  HAVE  BEEN  ENTERED  IN  EACH
ROUTINE
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C         DIMENSIONS  WHERE  STORAGE  SPACE  IS  SHORT.   THESE  CHANGES
MAY BE
C         MADE  TO  COVER  INCREASES  IN  THE  NUMBER  OF  PARAMETERS  PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------------
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION DYDC(NCPARM),DHDC(NCPARM),DGDC(NCPARM),DLYDC(2),
     1          DLHDC(2),DLGDC(2)
                          C   O   M   M   O   N       /   W   A   T   E   R   /
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1                     STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /SPACE/ DYDC,DHDC,DGDC,DLYDC,DLHDC,DLGDC,SC,TO,PT
C
-----------------------------------------------------------------------
C     CALCULATE THE APPROPRIATE TEMPERATURE TERM IN THE DERIVATIVE
C          AND RETURN.  --APPROPRIATE AS INDICATED BY J.
C
-----------------------------------------------------------------------
      GO TO (100,200,300,400,500,600,700,800,900,9999,
                                                    1
1100,1200,1300,1400,1500,1600,1700,1800,1900,9999),IGOES
  100 CONTINUE
C
-----------------------------------------------------------------------
C         THE DERIVATIVE FOR HEAT CAPACITY OF NON-IONIC SPECIES.
C
-----------------------------------------------------------------------
      DYDC(1)=ONE/(T*T*T)
```

```
      DYDC(2)=ONE/(T*T)
      DYDC(3)=ONE/T
      DYDC(4)=ONE/DSQRT(T)
      DYDC(5)=ONE
      DYDC(6)=T
      DYDC(7)=T*T
      DYDC(8)=T*T*T
      DYDC(9)=ZERO
      DYDC(10)=ZERO
      GO TO 1000
  200 CONTINUE
C
-----------------------------------------------------------------
C         THE DERIVATIVE FOR ENTROPY OF NON-IONIC SPECIES.
C
-----------------------------------------------------------------
      DYDC(1)=-ONE/(THREE*T*T*T)
      DYDC(2)=-ONE/(TWO*T*T)
      DYDC(3)=-ONE/T
      DYDC(4)=-TWO/DSQRT(T)
      DYDC(5)=DLOG(T)
      DYDC(6)=T
      DYDC(7)=T*T/TWO
      DYDC(8)=T*T*T/THREE
      DYDC(9)=ZERO
      DYDC(10)=ONE
      GO TO 1000
  300 CONTINUE
C
-----------------------------------------------------------------
C         THE DERIVATIVE FOR THE ENTHALPY OF NON-IONIC SPECIES.
C
-----------------------------------------------------------------
      DYDC(1)=-ONE/(TWO*T*T)
      DYDC(2)=-ONE/T
      DYDC(3)=DLOG(T)
      DYDC(4)=TWO*DSQRT(T)
      DYDC(5)=T
      DYDC(6)=T*T/TWO
      DYDC(7)=T*T*T/THREE
      DYDC(8)=T**4/FOUR
      DYDC(9)=ONE
      DYDC(10)=ZERO
      GO TO 1000
  400 CONTINUE
C
-----------------------------------------------------------------
C        THE DERIVATIVE FOR THE GIBBS ENERGY OF NON-IONIC SPECIES.
C
-----------------------------------------------------------------
      DYDC(1)=-ONE/(SIX*T*T)
      DYDC(2)=-ONE/(TWO*T)
      DYDC(3)=ONE+DLOG(T)
      DYDC(4)=FOUR*DSQRT(T)
```

```
      DYDC(5)=T-T*DLOG(T)
      DYDC(6)=-T*T/TWO
      DYDC(7)=-T*T*T/SIX
      DYDC(8)=-T**4/12.0D0
      DYDC(9)=ONE
      DYDC(10)=-T
      GO TO 1000
  500 CONTINUE
C
-----------------------------------------------------------------
C        THE DERIVATIVE FOR THE EQUILIBRIUM CONSTANT OF NON-IONIC
C             SPECIES.
C
-----------------------------------------------------------------
      DYDC(1)=ONE/(SIX*R*T*T*T)
      DYDC(2)=ONE/(TWO*R*T*T)
      DYDC(3)=-(ONE+DLOG(T))/(R*T)
      DYDC(4)=-FOUR/(R*DSQRT(T))
      DYDC(5)=-(ONE-DLOG(T))/R
      DYDC(6)=T/(TWO*R)
      DYDC(7)=T*T/(SIX*R)
      DYDC(8)=T*T*T/(12.0D0*R)
      DYDC(9)=-ONE/(R*T)
      DYDC(10)=ONE/R
      GO TO 1000
  600 CONTINUE
C
-----------------------------------------------------------------
C          THE DERIVATIVE FOR THE CELL POTENTIAL FOR NON-IONIC
SPECIES.
C
-----------------------------------------------------------------
      DYDC(1)=ONE/(SIX*F*T*T)
      DYDC(2)=ONE/(TWO*F*T)
      DYDC(3)=-(ONE+DLOG(T))/F
      DYDC(4)=-FOUR*DSQRT(T)/F
      DYDC(5)=-(T-T*DLOG(T))/F
      DYDC(6)=T*T/(TWO*F)
      DYDC(7)=T*T*T/(SIX*F)
      DYDC(8)=(T**4)/(12.0D0*F)
      DYDC(9)=-ONE/F
      DYDC(10)=T/F
      GO TO 1000
  700 CONTINUE
C
-----------------------------------------------------------------
C        THE DERIVATIVE FOR THE RELATIVE HEAT CONTENT OF NON-IONIC
C             SPECIES.
C
-----------------------------------------------------------------
      IF (SC.LT.ZERO)  GO TO 750
      DYDC(1)=-ONE/(TWO*T*T)
      DYDC(2)=-ONE/T
      DYDC(3)=DLOG(T)
```

```
      DYDC(4)=TWO*DSQRT(T)
      DYDC(5)=T
      DYDC(6)=T*T/TWO
      DYDC(7)=T*T*T/THREE
      DYDC(8)=T**4/FOUR
      DYDC(9)=ONE
      DYDC(10)=ZERO
      GO TO 1000
  750 CONTINUE
      DYDC(1)=-ONE/(TWO*TO*TO)
      DYDC(2)=-ONE/TO
      DYDC(3)=DLOG(TO)
      DYDC(4)=TWO*DSQRT(TO)
      DYDC(5)=TO
      DYDC(6)=TO*TO/TWO
      DYDC(7)=TO*TO*TO/THREE
      DYDC(8)=TO**4/FOUR
      DYDC(9)=ONE
      DYDC(10)=ZERO
      GO TO 1000
  800 CONTINUE
C
------------------------------------------------------------------
C      THE DERIVATIVE FOR THE GIBBS ENERGY FUNCTION OF NON-IONIC
SPECIES.
C
------------------------------------------------------------------
      DYDC(1)=ONE/(SIX*T**3)
      DYDC(2)=ONE/(TWO*T*T)
      DYDC(3)=-(ONE+DLOG(T))/T
      DYDC(4)=-FOUR/DSQRT(T)
      DYDC(5)=DLOG(T)-ONE
      DYDC(6)=T/TWO
      DYDC(7)=T*T/SIX
      DYDC(8)=T**3/12.0D0
      DYDC(9)=-ONE/T
      DYDC(10)=ONE
      GO TO 1000
  900 CONTINUE
      GO TO 9999
 1000 CONTINUE
      RETURN
 1100 CONTINUE
C
------------------------------------------------------------------
C         THE DERIVATIVE FOR THE HEAT CAPACITY OF IONIC SPECIES.
C
------------------------------------------------------------------
      DYDC(1)=ONE
      DYDC(2)=TWO*T
      DYDC(3)=ONE/(T*T)
      DYDC(4)=ZERO
      DYDC(5)=ZERO
      DYDC(6)=T*T
```

```
      FNT=FN(T)

DYDC(7)=-T*DIE(T)*(A*FNT*A*FNT+A*FNT*A+A*FNT*TWO/THETA+ONE/(THETA*
     1THETA))
      DYDC(8)=ZERO
      DYDC(9)=ZERO
      DYDC(10)=ZERO
      GO TO 2000
 1200 CONTINUE
C
-------------------------------------------------------------------
C          THE DERIVATIVE FOR THE ENTROPY OF IONIC SPECIES.
C
-------------------------------------------------------------------
      DYDC(1)=DLOG(T)
      DYDC(2)=TWO*T
      DYDC(3)=-ONE/(TWO*T*T)
      DYDC(4)=ZERO
      DYDC(5)=ZERO
      DYDC(6)=T*T/TWO
      DYDC(7)=-DIE(T)*(A*FN(T)+ONE/THETA)
      DYDC(8)=ZERO
      DYDC(9)=ZERO
      DYDC(10)=ONE
      GO TO 2000
 1300 CONTINUE
C
-------------------------------------------------------------------
C          THE DERIVATIVE FOR THE ENTHALPY OF IONIC SPECIES.
C
-------------------------------------------------------------------
      DYDC(1)=T
      DYDC(2)=T*T
      DYDC(3)=-ONE/T
      DYDC(4)=ZERO
      DYDC(5)=ZERO
      DYDC(6)=(T**3)/THREE
      DYDC(7)=DIE(T)*(ONE-A*T*FN(T)-T/THETA)
      DYDC(8)=ZERO
      DYDC(9)=ONE
      DYDC(10)=ZERO
      GO TO 2000
 1400 CONTINUE
C
-------------------------------------------------------------------
C          THE DERIVATIVE FOR THE GIBBS ENERGY OF IONIC SPECIES.
C
-------------------------------------------------------------------
      DYDC(1)=T-T*DLOG(T)
      DYDC(2)=-T*T
      DYDC(3)=-ONE/(TWO*T)
      DYDC(4)=ZERO
      DYDC(5)=ZERO
      DYDC(6)=-(T**3)/SIX
```

```
      DYDC(7)=DIE(T)
      DYDC(8)=ZERO
      DYDC(9)=ONE
      DYDC(10)=-T
      GO TO 2000
 1500 CONTINUE
C
-----------------------------------------------------------------
C         THE DERIVATIVE FOR THE EQUILIBRIUM CONSTANT OF IONIC
C             SPECIES.
C
-----------------------------------------------------------------
      DYDC(1)=(DLOG(T)-ONE)/R
      DYDC(2)=T/R
      DYDC(3)=ONE/(TWO*R*T*T)
      DYDC(4)=ZERO
      DYDC(5)=ZERO
      DYDC(6)=(T*T)/(SIX*R)
      DYDC(7)=-DIE(T)/(R*T)
      DYDC(7)=-DIE(T)/(R*T)
      DYDC(8)=ZERO
      DYDC(9)=-ONE/(R*T)
      DYDC(10)=ONE/R
      GO TO 2000
 1600 CONTINUE
C
-----------------------------------------------------------------
C         THE DERIVATIVE FOR THE CELL POTENTIAL OF IONIC SPECIES.
C
-----------------------------------------------------------------
      DYDC(1)=(T*DLOG(T)-T)/F
      DYDC(2)=(T*T)/F
      DYDC(3)=ONE/(TWO*F*T)
      DYDC(4)=ZERO
      DYDC(5)=ZERO
      DYDC(6)=(T**3)/(SIX*F)
      DYDC(7)=-DIE(T)/F
      DYDC(8)=ZERO
      DYDC(9)=-ONE/F
      DYDC(10)=T/F
      GO TO 2000
 1700 CONTINUE
C
-----------------------------------------------------------------
C         THE DERIVATIVE FOR THE RELATIVE HEAT CONTENT OF IONIC
C             SPECIES.
C
-----------------------------------------------------------------
      IF (SC.LT.0) GO TO 1750
      DYDC(1)=T
      DYDC(2)=T*T
      DYDC(3)=-ONE/T
      DYDC(4)=ZERO
      DYDC(5)=ZERO
```

```
      DYDC(6)=(T**3)/THREE
      DYDC(7)=DIE(T)*(ONE-A*T*FN(T)-T/THETA)
      DYDC(8)=ZERO
      DYDC(9)=ONE
      DYDC(10)=ZERO
      GO TO 2000
 1750 CONTINUE
      DYDC(1)=TO
      DYDC(2)=TO*TO
      DYDC(3)=-ONE/TO
      DYDC(4)=ZERO
      DYDC(5)=ZERO
      DYDC(6)=(TO**3)/THREE
      DYDC(7)=DIE(TO)*(ONE-A*TO*FN(TO)-TO/THETA)
      DYDC(8)=ZERO
      DYDC(9)=ONE
      DYDC(10)=ZERO
 2000 CONTINUE
      RETURN
C
-------------------------------------------------------------------
C     WRITE ERROR MESSAGE.
C
-------------------------------------------------------------------
 1800 CONTINUE
 1900 CONTINUE
 9999 CONTINUE
      WRITE (60,60)IGOES
      STOP
   60 FORMAT('0PROCESSING HAS STOPPED IN THE ROUTINE "YDERIV".'/'
IGOES
     1HAS  A  VALUE  OF  ',I5,'  BUT  THE  DERIVATIVES  ARE  NOT
AVAILABLE.')
      END
      SUBROUTINE HDERIV(T)
C
-------------------------------------------------------------------
C
C                              HDERIV
C
C     THIS VERSION WAS WRITEN 3/09/72 BY HAAS.
C          LAST REVISED 8/05/72 BY HAAS.
C
C       REVISED TO ACCEPT THE CODATA THERMAL FUNCTION BY HAAS,
8/31/84.
C
C
-------------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
C
-------------------------------------------------------------------
C
C       PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
```

```
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C         DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C         MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
------------------------------------------------------------------
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION DYDC(NCPARM),DHDC(NCPARM),DGDC(NCPARM),DLYDC(2),
     1          DLHDC(2),DLGDC(2)
                    C O M M O N       / W A T E R /
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1               STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /SPACE/ DYDC,DHDC,DGDC,DLYDC,DLHDC,DLGDC,SC,TO,PT
C
------------------------------------------------------------------
C     CALCULATE THE DERIVATIVE OF -D- WITH RESPECT TO THE OTHER
C          CONSTANTS WHERE THE ENTHALPY IS 0.0 AS IS THE
C          CASE FOR ELEMENTS AT 298.15 KELVIN.
C
------------------------------------------------------------------
      DHDC(1)=+ONE/(TWO*T*T)
      DHDC(2)=+ONE/T
      DHDC(3)=-DLOG(T)
      DHDC(4)=-TWO*DSQRT(T)
      DHDC(5)=-T
      DHDC(6)=-T*T/TWO
      DHDC(7)=-T*T*T/THREE
      DHDC(8)=-T**4/FOUR
      DHDC(9)=-ONE
      DHDC(10)=ZERO
      RETURN
      END
      SUBROUTINE GDERIV(T)
C
------------------------------------------------------------------
C
C                                      GDERIV
C
C     THIS VERSION WAS WRITEN 3/09/72 BY HAAS.
C          LAST REVISED 8/05/72 BY HAAS.
C
C       REVISED TO ACCEPT THE CODATA THERMAL FUNCTION BY HAAS,
8/31/84.
C
C
------------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
C
------------------------------------------------------------------
```

```
C
C      PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C       IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C        DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C        MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION DYDC(NCPARM),DHDC(NCPARM),DGDC(NCPARM),DLYDC(2),
     1          DLHDC(2),DLGDC(2)
                     COMMON      /WATER/
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1                STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /SPACE/ DYDC,DHDC,DGDC,DLYDC,DLHDC,DLGDC,SC,TO,PT
C
-----------------------------------------------------------------
C     CALCULATE THE DERIVATIVE OF -D- WITH RESPECT TO THE OTHER
C          CONSTANTS WHERE THE GIBBS ENERGY IS 0.0 AS IS THE
C          CASE FOR PHASES AT THE TEMPERATURE OF INVERSION.
C
-----------------------------------------------------------------
      DGDC(1)=ONE/(SIX*T*T)
      DGDC(2)=ONE/(TWO*T)
      DGDC(3)=-(ONE+DLOG(T))
      DGDC(4)=-FOUR*DSQRT(T)
      DGDC(5)=T*DLOG(T)-T
      DGDC(6)=T*T/TWO
      DGDC(7)=T*T*T/SIX
      DGDC(8)=T**4/12.0D0
      DGDC(9)=-ONE
      DGDC(10)=T
      RETURN
      END
      SUBROUTINE LYDRIV(T,IGOES,INDEX,JL,JH,JT)
C
-----------------------------------------------------------------
C
C     "LYDRIV" CALCULATES THE DERIVATIVES FOR THE LAMBDA ANOMALY
C       FUNCTIONS WITH RESPECT TO THE CONSTANTS A13, AND A14.  FOR

C            FURTHER INFORMATION REFER TO INDEN, 1981, PHYSICA,
103B:82-100.
C
C     LAST REVISED 1 DEC 1988 BY HAAS.
C
-----------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
```

```
      REAL*8 LNTAU
C
-----------------------------------------------------------------
C
C       PARAMETERS  STATEMENTS.   THESE  HAVE  BEEN  ENTERED  IN  EACH
ROUTINE
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C         DIMENSIONS  WHERE  STORAGE  SPACE  IS  SHORT.   THESE  CHANGES
MAY BE
C         MADE  TO  COVER  INCREASES  IN  THE  NUMBER  OF  PARAMETERS  PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------
                           D    I    M    E    N    S    I    O    N
X(NX,IP2),P(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1         ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION DYDC(NCPARM),DHDC(NCPARM),DGDC(NCPARM),DLYDC(2),
     1         DLHDC(2),DLGDC(2)
      COMMON /AIR/ X,P,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1            ISING,ISTOP,IL,JDF,ION
                   C    O    M    M    O    N       /    W    A    T    E    R    /
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1              STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /SPACE/ DYDC,DHDC,DGDC,DLYDC,DLHDC,DLGDC,SC,TO,PT
      TC=P(INDEX+NCPARM)*(0.1d0*P(INDEX+NCPARM+1)*(PT-PREF)+1.D0)
      TAU=T/TC
      LNTAU=DLOG(TAU)
      AJL=DBLE(FLOAT(JL))
      AJH=DBLE(FLOAT(-JH))
      DLYDC(1)=ZERO
      DLYDC(2)=ZERO
      GO TO (1000,2000,3000,4000,5000,6000,7000), IGOES
C
-----------------------------------------------------------------
C        DERIVATIVE OF THE LAMBDA ANOMALY FUNCTION WITH RESPECT TO
C           THE  CONSTANTS  FOR  THE  TWO  LIMBS  OF  THE  HEAT  CAPACITY
EQUATION.
C
-----------------------------------------------------------------
 1000 CONTINUE
      DO 1200 I=1,JT
      ITERM=2*I-1
      AITERM=DBLE(FLOAT(ITERM))
      IF(T.GT.TC)  GO TO 1100
      EXPON=AJL*AITERM
      DLYDC(1)=DLYDC(1)+DEXP(LNTAU*EXPON)/AITERM
      GO TO 1200
 1100 CONTINUE
      EXPON=AJH*AITERM
```

```
      DLYDC(2)=DLYDC(2)+DEXP(LNTAU*EXPON)/AITERM
 1200 CONTINUE
      RETURN
C
-----------------------------------------------------------------------
C         DERIVATIVE OF THE LAMBDA ANOMALY FUNCTION WITH RESPECT TO
C          THE CONSTANTS FOR THE TWO LIMBS OF THE ENTROPY EQUATION.
C
-----------------------------------------------------------------------
 2000 CONTINUE
      DO 2200 I=1,JT
      ITERM=2*I-1
      AITERM=DBLE(FLOAT(ITERM))
      IF(T.GT.TC)  GO TO 2100
      EXPON=AJL*AITERM
      DLYDC(1)=DLYDC(1)+DEXP(LNTAU*EXPON)/(EXPON*AITERM)
      GO TO 2200
 2100 CONTINUE
      EXPON=AJH*AITERM
      DLYDC(2)=DLYDC(2)+DEXP(LNTAU*EXPON)/(EXPON*AITERM)
      DLYDC(1)=DLYDC(1)+ONE/(AJL*AITERM*AITERM)
      DLYDC(2)=DLYDC(2)-ONE/(AJH*AITERM*AITERM)
 2200 CONTINUE
      RETURN
C
-----------------------------------------------------------------------
C         DERIVATIVE OF THE LAMBDA ANOMALY FUNCTION WITH RESPECT TO
C         THE CONSTANTS FOR THE TWO LIMBS OF THE ENTHALPY EQUATION.
C
-----------------------------------------------------------------------
 3000 CONTINUE
      DO 3200 I=1,JT
      ITERM=2*I-1
      AITERM=DBLE(FLOAT(ITERM))
      IF(T.GT.TC)  GO TO 3100
      EXPON=AJL*AITERM+ONE
      DLYDC(1)=DLYDC(1)+DEXP(LNTAU*EXPON)/(AITERM*EXPON)
      GO TO 3200
 3100 CONTINUE
      EXPON=AJH*AITERM+ONE
      DLYDC(2)=DLYDC(2)+DEXP(LNTAU*EXPON)/(AITERM*EXPON)
      DLYDC(1)=DLYDC(1)+ONE/(AITERM*(AJL*AITERM+ONE))
      DLYDC(2)=DLYDC(2)-ONE/(AITERM*(AJH*AITERM+ONE))
 3200 CONTINUE
      DLYDC(1)=TC*DLYDC(1)
      DLYDC(2)=TC*DLYDC(2)
      RETURN
C
-----------------------------------------------------------------------
C         DERIVATIVE OF THE LAMBDA ANOMALY FUNCTION WITH RESPECT TO
C            THE CONSTANTS FOR THE TWO LIMBS OF THE GIBBS ENERGY
EQUATION.
C
-----------------------------------------------------------------------
```

```
 4000 CONTINUE
      DO 4200 I=1,JT
      ITERM=2*I-1
      AITERM=DBLE(FLOAT(ITERM))
      IF(T.GT.TC)  GO TO 4100
      EXPON=AJL*AITERM+ONE
      EXPON2=AJL*AITERM
      DLYDC(1)=DLYDC(1)+TC*DEXP(LNTAU*EXPON)/(AITERM*EXPON)
     1              -T*DEXP(LNTAU*EXPON2)/(EXPON2*AITERM)
      GO TO 4200
 4100 CONTINUE
      EXPON=AJH*AITERM+ONE
      EXPON2=AJH*AITERM
      DLYDC(2)=DLYDC(2)+TC*DEXP(LNTAU*EXPON)/(AITERM*EXPON)
     1              -T*DEXP(LNTAU*EXPON2)/(EXPON2*AITERM)
      DLYDC(1)=DLYDC(1)+TC/(AITERM*(AJL*AITERM+ONE))
     1              -T/(AJL*AITERM*AITERM)
      DLYDC(2)=DLYDC(2)-TC/(AITERM*(AJH*AITERM+ONE))
     1              +T/(AJH*AITERM*AITERM)
 4200 CONTINUE
      RETURN
C
----------------------------------------------------------------
C        DERIVATIVE OF THE LAMBDA ANOMALY FUNCTION WITH RESPECT TO
C           THE CONSTANTS FOR THE TWO LIMBS OF THE EQUILIBRIUM
CONSTANT EQUATION.
C
----------------------------------------------------------------
 5000 CONTINUE
      DO 5200 I=1,JT
      ITERM=2*I-1
      AITERM=DBLE(FLOAT(ITERM))
      IF(T.GT.TC)  GO TO 5100
      EXPON=AJL*AITERM+ONE
      EXPON2=AJL*AITERM
      DLYDC(1)=DLYDC(1)+TC*DEXP(LNTAU*EXPON)/(AITERM*EXPON)
     1              -T*DEXP(LNTAU*EXPON2)/(EXPON2*AITERM)
      GO TO 5200
 5100 CONTINUE
      EXPON=AJH*AITERM+ONE
      EXPON2=AJH*AITERM
      DLYDC(2)=DLYDC(2)+TC*DEXP(LNTAU*EXPON)/(AITERM*EXPON)
     1              -T*DEXP(LNTAU*EXPON2)/(EXPON2*AITERM)
      DLYDC(1)=DLYDC(1)+TC/(AITERM*(AJL*AITERM+ONE))
     1              -T/(AJL*AITERM*AITERM)
      DLYDC(2)=DLYDC(2)-TC/(AITERM*(AJH*AITERM+ONE))
     1              +T/(AJH*AITERM*AITERM)
 5200 CONTINUE
      DLYDC(1)=-DLYDC(1)/(R*T)
      DLYDC(2)=-DLYDC(2)/(R*T)
      RETURN
C
----------------------------------------------------------------
C        DERIVATIVE OF THE LAMBDA ANOMALY FUNCTION WITH RESPECT TO
```

```
C         THE CONSTANTS FOR THE TWO LIMBS OF THE EMF EQUATION.
C
------------------------------------------------------------------
 6000 CONTINUE
      DO 6200 I=1,JT
      ITERM=2*I-1
      AITERM=DBLE(FLOAT(ITERM))
      IF(T.GT.TC)  GO TO 6100
      EXPON=AJL*AITERM+ONE
      EXPON2=AJL*AITERM
      DLYDC(1)=DLYDC(1)+TC*DEXP(LNTAU*EXPON)/(AITERM*EXPON)
     1              -T*DEXP(LNTAU*EXPON2)/(EXPON2*AITERM)
      GO TO 6200
 6100 CONTINUE
      EXPON=AJH*AITERM+ONE
      EXPON2=AJH*AITERM
      DLYDC(2)=DLYDC(2)+TC*DEXP(LNTAU*EXPON)/(AITERM*EXPON)
     1              -T*DEXP(LNTAU*EXPON2)/(EXPON2*AITERM)
      DLYDC(1)=DLYDC(1)+TC/(AITERM*(AJL*AITERM+ONE))
     1              -T/(AJL*AITERM*AITERM)
      DLYDC(2)=DLYDC(2)-TC/(AITERM*(AJH*AITERM+ONE))
     1              +T/(AJH*AITERM*AITERM)
 6200 CONTINUE
      DLYDC(1)=-DLYDC(1)/F
      DLYDC(2)=-DLYDC(2)/F
      RETURN
C
------------------------------------------------------------------
C        DERIVATIVE OF THE LAMBDA ANOMALY FUNCTION WITH RESPECT TO
C           THE CONSTANTS FOR THE TWO LIMBS OF THE HEAT CONTENT
EQUATION.
C
------------------------------------------------------------------
 7000 CONTINUE
      IF(SC.GE.0.D0)  GO TO 7050
      TAU=TO/TC
      LNTAU=DLOG(TAU)
 7050 CONTINUE
      DO 7200 I=1,JT
      ITERM=2*I-1
      AITERM=DBLE(FLOAT(ITERM))
      IF(TAU.GT.ONE)  GO TO 7100
      EXPON=AJL*AITERM+ONE
      DLYDC(1)=DLYDC(1)+DEXP(LNTAU*EXPON)/(AITERM*EXPON)
      GO TO 7200
 7100 CONTINUE
      EXPON=AJH*AITERM+ONE
      DLYDC(2)=DLYDC(2)+DEXP(LNTAU*EXPON)/(AITERM*EXPON)
      DLYDC(1)=DLYDC(1)+ONE/(AITERM*(AJL*AITERM+ONE))
      DLYDC(2)=DLYDC(2)-ONE/(AITERM*(AJH*AITERM+ONE))
 7200 CONTINUE
      DLYDC(1)=TC*DLYDC(1)
      DLYDC(2)=TC*DLYDC(2)
      RETURN
```

```
      END
      SUBROUTINE LHDRIV(T,INDEX,JL,JH,JT)
C
-----------------------------------------------------------------------
C
C     "LHDRIV" CALCULATES THE DERIVATIVES FOR THE LAMBDA ANOMALY
C        FUNCTION WITH RESPECT TO THE CONSTANTS A13 AND A14 WHERE
THE
C        PHASE IS A REFERENCE PHASE AND THE ENTHALPY OF FORMATION
IS
C        ZERO.
C
C     LAST REVISED 1 DEC 1988 BY HAAS.
C
-----------------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 LNTAU
C
-----------------------------------------------------------------------
C
C       PARAMETERS STATEMENTS.   THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C         IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C         DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C         MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C         ALSO.
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------------
                          D   I   M   E   N   S   I   O   N
X(NX,IP2),P(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1          ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION DYDC(NCPARM),DHDC(NCPARM),DGDC(NCPARM),DLYDC(2),
     1          DLHDC(2),DLGDC(2)
      COMMON /AIR/ X,P,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1             ISING,ISTOP,IL,JDF,ION
                   C   O   M   M   O   N     /   W   A   T   E   R   /
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1               STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /SPACE/ DYDC,DHDC,DGDC,DLYDC,DLHDC,DLGDC,SC,TO,PT
      TC=P(INDEX+NCPARM)*(0.1d0*P(INDEX+NCPARM+1)*(PT-PREF)+1.D0)
      TAU=T/TC
      LNTAU=DLOG(TAU)
      AJL=DBLE(FLOAT(JL))
      AJH=DBLE(FLOAT(-JH))
      DLHDC(1)=ZERO
      DLHDC(2)=ZERO
      DO 2000 I=1,JT
      ITERM=2*I-1
```

```
      AITERM=DBLE(FLOAT(ITERM))
      IF(T.GT.TC)  GO TO 1000
      EXPON=AJL*AITERM+ONE
      DLHDC(1)=DLHDC(1)-DEXP(LNTAU*EXPON)/(AITERM*EXPON)
      GO TO 2000
 1000 CONTINUE
      EXPON=AJH*AITERM+ONE
      DLHDC(2)=DLHDC(2)-DEXP(LNTAU*EXPON)/(AITERM*EXPON)
      DLHDC(1)=DLHDC(1)-ONE/(AITERM*(AJL*AITERM+ONE))
      DLHDC(2)=DLHDC(2)+ONE/(AITERM*(AJH*AITERM+ONE))
 2000 CONTINUE
      DLHDC(1)=TC*DLHDC(1)
      DLHDC(2)=TC*DLHDC(2)
      RETURN
      END
      SUBROUTINE LGDRIV(T,INDEX,JL,JH,JT)
C
-----------------------------------------------------------------------
C
C     "LGDRIV" CALCULATES THE DERIVATIVES FOR THE LAMBDA ANOMALY
C        FUNCTION WITH RESPECT TO THE CONSTANTS A13 AND A14 WHERE
THE
C       GIBBS ENERGY DIFFERENCE AT THE TEMPERATURE OF INVERSION IS
C        SET TO 0.D0.
C
C     LAST REVISED 1 DEC 1988 BY HAAS.
C
-----------------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
      REAL*8 LNTAU
C
-----------------------------------------------------------------------
C
C      PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C       IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C        DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C        MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------------
                                  D   I   M   E   N   S   I   O   N
X(NX,IP2),P(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1          ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION DYDC(NCPARM),DHDC(NCPARM),DGDC(NCPARM),DLYDC(2),
     1          DLHDC(2),DLGDC(2)
      COMMON /AIR/ X,P,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1             ISING,ISTOP,IL,JDF,ION
```

```
                    C O M M O N       / W A T E R /
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1                 STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /SPACE/ DYDC,DHDC,DGDC,DLYDC,DLHDC,DLGDC,SC,TO,PT
      TC=P(INDEX+NCPARM)*(0.1d0*P(INDEX+NCPARM+1)*(PT-PREF)+1.D0)
      TAU=T/TC
      LNTAU=DLOG(TAU)
      AJL=DBLE(FLOAT(JL))
      AJH=DBLE(FLOAT(-JH))
      DLGDC(1)=ZERO
      DLGDC(2)=ZERO
      DO 2000 I=1,JT
      ITERM=2*I-1
      AITERM=DBLE(FLOAT(ITERM))
      IF(T.GT.TC)  GO TO 1000
      EXPON=AJL*AITERM+ONE
      EXPON2=AJL*AITERM
      DLGDC(1)=DLGDC(1)-TC*DEXP(LNTAU*EXPON)/(AITERM*EXPON)
     1              +T*DEXP(LNTAU*EXPON2)/(EXPON2*AITERM)
      GO TO 2000
 1000 CONTINUE
      EXPON=AJH*AITERM+ONE
      EXPON2=AJH*AITERM
      DLGDC(2)=DLGDC(2)-TC*DEXP(LNTAU*EXPON)/(AITERM*EXPON)
     1              +T*DEXP(LNTAU*EXPON2)/(EXPON2*AITERM)
      DLGDC(1)=DLGDC(1)-TC/(AITERM*(AJL*AITERM+ONE))
     1              +T/(AJL*AITERM*AITERM)
      DLGDC(2)=DLGDC(2)+TC/(AITERM*(AJH*AITERM+ONE))
     1              -T/(AJH*AITERM*AITERM)
 2000 CONTINUE
      RETURN
      END
      FUNCTION GEF(T,J)
C
-----------------------------------------------------------------
C
C      "GEF" RETURNS THE GIBBS ENERGY FUNCTION FOR THE REACTION
GIVEN IN
C        THE "J-TH" DATA SET.
C
C     FOR A DISCUSSION OF THE "THIRD-LAW" TEST OF A DATA SET, REFER
C        TO :
C          CHASE AND OTHERS (1985), JANAF THERMOCHEMICAL TABLES,
JOURNAL
C               OF PHYSICAL AND CHEMICAL REFERENCE DATA, V 14,
SUPPLEMENT
C           #1  (ESPECIALLY REFER TO PAGE 13FF, SECTION ENTITLED
C            "EVALUATION OF THERMODYNAMIC DATA".)
C
C     LAST REVISED 1 DEC 1988 BY HAAS.
C
-----------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
C
```

```
-----------------------------------------------------------------
C
C       PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C         DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C         MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
-----------------------------------------------------------------
      GEF=FNCALC(T,J,8)
      RETURN
      END
      FUNCTION PTGEF(T,P,J)
C
-----------------------------------------------------------------
C
C      "PTGEF" CALCULATES THE GIBBS ENERGY DIFFERENCE BETWEEN "P"
AND
C        "PO(=PREF)" AT T, THE TEMPERATURE OF THE OBSERVATION.
C       THE FUNCTION IS NEEDED TO CORRECT THE GIBBS ENERGY TO "PO"
SO
C        THAT THE THIRD-LAW ENTHALPY OF REACTION CAN BE CALCULATED
AT
C         TREF.  THE CALCULATION IS DEPENDENT ONLY ON THE CURRENT
VALUES
C        FOR THE VOLUME OF THE PHASES INVOLVED.
C
C     WRITTEN 6/82 BY HAAS.
C
C
-----------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
      LOGICAL*1 LAMBDA,NOLAM,UNDAMP
      REAL*8 KBM,INTVDP
C
-----------------------------------------------------------------
C
C       PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C         DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C         MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
```

```
C
-----------------------------------------------------------------
      DIMENSION COEF(IP4,IP3),TINV(IP4,IP3,IP10),NPHASE(IP3),
                1
IKOUNT(IP3),IGO(IP3),ISTATE(IP4,IP3),INSTAT(IP4,IP3),
     2        INVPH(IP4,IP3,IP11),INVSC(IP4,IP3),ISPECL(IP4,IP3),
     3          IPHASE(IP4,IP3),NINVER(IP4,IP3)
                            DIMENSION
X(NX,IP2),PC(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1         ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION DYDC(NCPARM),DHDC(NCPARM),DGDC(NCPARM),DLYDC(2),
     1          DLHDC(2),DLGDC(2)
      DIMENSION LAMBDA(IP1),NOLAM(IP4,IP3)
      COMMON /EARTH/ COEF,TINV,NPHASE,IKOUNT,IGO,ISTATE,INSTAT,
     1               INVPH,INVSC,ISPECL,IPHASE,NINVER,NSETS,LISTP
      COMMON /AIR/ X,PC,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1             ISING,ISTOP,IL,JDF,ION
                    COMMON /WATER/
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1               STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /SPACE/ DYDC,DHDC,DGDC,DLYDC,DLHDC,DLGDC,SC,TO,PT
      COMMON /AETHER/ LAMBDA,NOLAM,UNDAMP
C
-----------------------------------------------------------------
C     INITIALIZE CONSTANTS.
C
-----------------------------------------------------------------
      Y=0.0D0
      PO=PREF
      LAST=NPHASE(J)
      DO 3000 L=1,LAST
      ACOEF=COEF(L,J)
      ITEM=NCPARM+NMPARM+NPARM*(IPHASE(L,J)-1)+1
      B1=PC(ITEM)
      B2=PC(ITEM+1)
      B3=PC(ITEM+2)
      B4=PC(ITEM+3)
      B5=PC(ITEM+4)
      B6=PC(ITEM+5)
      VR=PC(ITEM+6)
      DEBT=PC(ITEM+7)
      RTT=DEXP(-T/DEBT)
      IF(NOLAM(L,J))  GO TO 1000
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 1000
      A12=PC(ITEM-3)
      TC=PC(ITEM-4)*(0.1d0*PC(ITEM-3)*(P-PREF)+ONE)
      PT=P
      A13=PC(ITEM-2)
      A14=PC(ITEM-1)
      TAU=T/TC
      JL=PC(ITEM+8)
      JH=PC(ITEM+9)
      JT=PC(ITEM+10)
```

```
 1000 CONTINUE
C
------------------------------------------------------------------
C     CALCULATE THE VOLUME VT AT P=0.0 BARS.
C
------------------------------------------------------------------
      Z=B1*T+B2*T*T/TWO-DEBT*B3*RTT
      VRZ=VR*DEXP(Z)
      VT=VRZ
      IF(NOLAM(L,J))  GO TO 2000
      IF(.NOT.LAMBDA(IPHASE(L,J)))  GO TO 2000
      CALL LYDRIV(T,3,INDEX,JL,JH,JT)
      VT=VT+A12*A13*DLYDC(1)
      IF(TAU.LE.ONE)  GO TO 2000
      VT=VT+A12*A14*DLYDC(2)
 2000 CONTINUE
C
------------------------------------------------------------------
C     CALCULATE THE INTEGRAL {V*dP} FROM PO TO P.
C
------------------------------------------------------------------
      KBM=B4+B5*T
      U=ONE+B6*P/KBM
      UO=ONE+B6*PO/KBM
      W=-ONE/B6
      UWP1=U**(W+ONE)
      UOWP1=UO**(W+ONE)
      INTVDP=KBM*(UWP1-UOWP1)/(B6-ONE)
      Y=Y+0.1D0*ACOEF*VT*INTVDP
 3000 CONTINUE
      PTGEF=Y
C
------------------------------------------------------------------
C     RETURN TO CALLING PROGRAM.
C
------------------------------------------------------------------
      RETURN
      END
      SUBROUTINE PUTOUT(J)
      IMPLICIT REAL*8(A-H,O-Z)
      CHARACTER*23 DATE
      CHARACTER*1 BCD,LABEL
      CHARACTER*8 PNAME,TITLE,REF,RECKON,UNITS,YESNO,TYPE,ASTAR
      LOGICAL*1 LAMBDA,NOLAM,UNDAMP
      REAL*4 ACOEF
C
------------------------------------------------------------------
C
C       PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C         DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
MAY BE
C         MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
```

```
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
-------------------------------------------------------------------
      DIMENSION SGN(2),A(IP5,NPARM)
      DIMENSION COEF(IP4,IP3),TINV(IP4,IP3,IP10),NPHASE(IP3),
               1
IKOUNT(IP3),IGO(IP3),ISTATE(IP4,IP3),INSTAT(IP4,IP3),
     2        INVPH(IP4,IP3,IP11),INVSC(IP4,IP3),ISPECL(IP4,IP3),
     3          IPHASE(IP4,IP3),NINVER(IP4,IP3)
                           DIMENSION
X(NX,IP2),P(IP6),DC(IP6),YO(IP2),SIGYO(IP2),SIGYON(IP2)
     1         ,PD(IP6),KI(IP6),ION(IP1)
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
      DIMENSION DYDC(NCPARM),DHDC(NCPARM),DGDC(NCPARM),DLYDC(2),
     1          DLHDC(2),DLGDC(2)
      DIMENSION AA(IP6)
      DIMENSION PNAME(IP1),TITLE(10),REF(20,IP3),UNITS(4),YESNO(2),
     1          TYPE(IP9),LABEL(50)
      DIMENSION LAMBDA(IP1),NOLAM(IP4,IP3)
C
-------------------------------------------------------------------
C     COMMON BLOCKS
C
-------------------------------------------------------------------
      COMMON /EARTH/ COEF,TINV,NPHASE,IKOUNT,IGO,ISTATE,INSTAT,
     1              INVPH,INVSC,ISPECL,IPHASE,NINVER,NSETS,LISTP
      COMMON /AIR/ X,P,DC,YO,SIGYO,SIGYON,PD,KI,NC,IC,NV,IW,NP,NO,
     1            ISING,ISTOP,IL,JDF,ION
                           COMMON       /WATER/
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,AV,SCINV,TREF,PREF,
     1              STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      COMMON /TIME_/ DATE_
      COMMON /SPACE/ DYDC,DHDC,DGDC,DLYDC,DLHDC,DLGDC,SC,TO,PT
      COMMON /MAN/ AA
      COMMON /HOTAIR/ PNAME,TITLE,REF,UNITS,RECKON,YESNO,ASTAR,
     1               TYPE,LABEL,BCD
      COMMON /AETHER/ LAMBDA,NOLAM,UNDAMP
      SAVE
      CPRIME=ZERO
      LSTPHA=NPHASE(J)
      DO 1200 L=1,LSTPHA
      INDEX=1+NPARM*(IPHASE(L,J)-1)
      D=0.0D0
      IF (ISTATE(L,J).NE.1) GO TO 200
      CALL HDERIV(TREF)
      DO 100 K=1,NCPARM
      D=D+P(INDEX+K-1)*DGDC(K)
  100 CONTINUE
      GO TO 900
  200 CONTINUE
```

```
      IF (NINVER(L,J).EQ.0) GO TO 900
      DO 300 I=1,2
      SGN(I)=SCINV(I)
  300 CONTINUE
      IF (INVSC(L,J).EQ.0) GO TO 500
      DO 400 LLL=1,2
      SGN(LLL)=SGN(LLL)*STCOEF(INVSC(L,J))
  400 CONTINUE
  500 CONTINUE
      IF (INSTAT(L,J).EQ.0) GO TO 700
      INDEX2=1+NPARM*(INVPH(L,J,1)-1)
      CALL HDERIV(TREF)
      DO 600 K=1,NCPARM
      D=D+P(INDEX2+K-1)*DGDC(K)*SGN(2)
  600 CONTINUE
  700 CONTINUE
      LSTINV=NINVER(L,J)
      DO 800 LST=1,LSTINV
        IF    ((LST.EQ.LSTINV).AND.(INVSC(L,J).NE.0))
SGN(2)=SGN(2)/STCOEF(IN
     1VSC(L,J))
      CALL GDERIV(TINV(L,J,LST))
      DO 800 LLL=1,2
      INDEX2=1+NPARM*(INVPH(L,J,LST+LLL-1)-1)
      DO 800 K=1,NCPARM
      D=D+P(INDEX2+K-1)*DGDC(K)*SGN(LLL)
  800 CONTINUE
  900 CONTINUE
      DO 1000 K=1,NPARM
      A(L,K)=P(INDEX+K-1)
 1000 CONTINUE
      A(L,9)=A(L,9)+D
      DO 1100 K=1,NPARM
      AA(INDEX+K-1)=A(L,K)
 1100 CONTINUE
 1200 CONTINUE
      LST=LSTPHA+1
      DO 1300 K=1,NPARM
      A(LST,K)=0.0D0
 1300 CONTINUE
      DO 1500 L=1,LSTPHA
      DO 1500 K=1,NPARM
      IF ((K.EQ.7).AND.(ISTATE(L,J).EQ.-1)) GO TO 1400
      A(LST,K)=A(LST,K)+A(L,K)*COEF(L,J)
      GO TO 1500
 1400 CPRIME=CPRIME+A(L,K)*COEF(L,J)
 1500 CONTINUE
      RETURN
      ENTRY PUTIT (J)
      WRITE (3,1900) DATE
      DO 1600 L=1,LSTPHA
      ACOEF=COEF(L,J)
      WRITE (3,2000) PNAME(IPHASE(L,J)),ACOEF,(A(L,K),K=1,NPARM)
 1600 CONTINUE
```

```
      IF ((NPHASE(J).EQ.1).OR.((IGO(J).GE.7).AND.(IGO(J).NE.28)))
     1   GO TO 1800
      IF (CPRIME.EQ.ZERO) GO TO 1700
      WRITE (3,2200)
      WRITE (3,2300) (A(LST,K),K=1,NPARM),CPRIME
      GO TO 1800
 1700 CONTINUE
      WRITE (3,2200)
      WRITE (3,2300) (A(LST,K),K=1,NPARM)
 1800 CONTINUE
      RETURN
     1    9    0    0             F    O    R    M    A    T
(1H0,A23,10H----------/6H0PHASE,8X,4HCOEF,9X,9HC(1/7/13),
                                                                 1
9X,9HC(2,8,14),9X,9HC(3,9,15),9X,10HC(4,10,16),8X,10HC(5,11,17)
     1  8X,10HC(6,12,18))
 2000 FORMAT (1H0,A8,4X,F6.3,1X,1P6D18.7/(1h ,19X,1P6D18.7))
 2100 FORMAT (1H0/1H ,26X,9HC(1/7/13),
                                                                 1
9X,9HC(2,8,14),9X,9HC(3,9,15),9X,10HC(4,10,16),8X,10HC(5,11,17)
     1  8X,10HC(6,12,18))
 2200 FORMAT (1H0/1H ,26X,9HC(1/7/13),
                                                                 1
9X,9HC(2,8,14),9X,9HC(3,9,15),9X,10HC(4,10,16),8X,10HC(5,11,17)
     1  8X,10HC(6,12,18))
 2300 FORMAT (20H0REACTION CONSTANTS ,1P6D18.7/(1H ,19X,1P6D18.7))
      END
      SUBROUTINE PRPLOT
C
-----------------------------------------------------------------
C
C          MODIFIED TO BE RUN WITH <PHAS20> BY HAAS.
C
C
-----------------------------------------------------------------
      IMPLICIT LOGICAL(W), LOGICAL(K)
      DIMENSION  NSCALE(5), ABNOS(26), X(1), Y(1)
      CHARACTER*1 NOS(10)
      CHARACTER*1 WL
      CHARACTER*1 IMAGE(5000),CH,LABEL(50)
      CHARACTER*1 VC,HC,FOR1(19),FOR2(15),FOR3(19),NC,BL,HF,HF1
      CHARACTER*19 FOX1,FOX3
      CHARACTER*15 FOX2
      CHARACTER*1 VCR
      EQUIVALENCE (VC,VCR)
      SAVE
      DATA NOS/'0','1','2','3','4','5','6','7','8','9'/
      DATAHC/'-'/,NC/'+'/,BL/' '/,HF/'F'/,HF1/'.'/
C     DATA FOX1/24H(1XA1,F9.2,  121A1)      /
C     DATA FOX2/24H(1XA1, 9X121A1)          /
C     DATA FOX3/24H(1H0F   . ,   F   . )    /
      DATA FOR1/'(','1','X','A','1',',','F','9','.','2',',',' ','
',
     1  '1','2','1','A','1',')'/
```

```
         DATA  FOR2/'(','1','X','A','1',',','
','9','X','1','2','1','A',
     1  '1',')'/
      DATA FOR3/'(','1','H','0','F',' ',' ','.',' ',',',' ',' ',
     1  'F',' ',' ',' ','.',' ',')'/
      DATA VCR/'¦'/
      DATA KPLOT1/.FALSE./,KPLOT2/.FALSE./
      DATA KABSC,KORD,KBOTGL/3*.FALSE./
C
      ENTRY PLOT1 (NSCALE,NHL,NSBH,NVL,NSBV)
      KPLOT1=.TRUE.
      KPLOT2=.FALSE.
      NH=IABS(NHL)
      NSH=IABS(NSBH)
      NV=IABS(NVL)
      NSV=IABS(NSBV)
      NSCL=NSCALE(1)
      IF (NH*NSH*NV*NSV.NE.0) GO TO 200
      WRITE (60,100)
100      FORMAT (T5,'SOME PLOT1 ARG. ILLEGALLY 0')
      KPLOT=.FALSE.
      RETURN
200      KPLOT=.TRUE.
      IF (NV.LE.25) GO TO 400
      WRITE (60,300)
      KPLOT=.FALSE.
300      FORMAT (T5,'NO. OF VERTICAL LINES >25')
      RETURN
400      CONTINUE
      NVP=NV+1
      NDH=NH*NSH
      NDHP=NDH+1
      NDV=NV*NSV
      NDVP=NDV+1
      NIMG=(NDHP*NDVP)
      IF (NDV.LE.120) GO TO 600
      KPLOT=.FALSE.
      WRITE (60,500)
500      FORMAT (T5,'WIDTH OF GRAPH >121')
      RETURN
600      CONTINUE
      IF (NSCL.EQ.0) GO TO 700
          FSY=10.**NSCALE(2)
          FSX=10.**NSCALE(4)
          IY=MIN0(IABS(NSCALE(3)),7)+1
          IX=MIN0(IABS(NSCALE(5)),9)+1
      GO TO 800
700      FSY=1.
      FSX=1.
      IY=4
      IX=4
800      FOR1(10)=NOS(IY)
      NA=MIN0(IX,NSV)-1
      NS=NA-MIN0(NA,120-NDV)
```

```
      NB=11-NS+NA
      I1=NB/10
      I2=NB-I1*10
      FOR3(6)=NOS(I1+1)
      FOR3(7)=NOS(I2+1)
      FOR3(9)=NOS(NA+1)
      IF (NV.GT.0) GO TO 1000
      DO 900 J=11,18
900      FOR3(J)=BL
      GO TO 1100
1000      I1=NV/10
      I2=NV-I1*10
      FOR3(11)=NOS(I1+1)
      FOR3(12)=NOS(I2+1)
      FOR3(13)=HF
      I1=NSV/100
      I3=NSV-I1*100
      I2=I3/10
      I3=I3-I2*10
      FOR3(14)=NOS(I1+1)
      FOR3(15)=NOS(I2+1)
      FOR3(16)=NOS(I3+1)
      FOR3(17)=HF1
      FOR3(18)=FOR3(9)
1100      CONTINUE
c      ENCODE (19,3400,FOX1)(FOR1(I),I=1,19)
c      ENCODE (15,3500,FOX2) (FOR2(I),I=1,15)
c      ENCODE (19,3400,FOX3) (FOR3(I),I=1,19)
C  DG.    THE ENCODE STATEMENTS, ABOVE, WERE REPLACE WITH INTERNAL
WRITES
C    FROM FOR TO FOX
       WRITE(UNIT=FOX1(1:19),FMT=3400)(FOR1(I),I=1,19)
       WRITE(UNIT=FOX2(1:15),FMT=3500)(FOR2(I),I=1,15)
       WRITE(UNIT=FOX3(1:19),FMT=3400)(FOR3(I),I=1,19)
c
      IF (KPLOT1) RETURN
      KPLOT1=.TRUE.
C
      ENTRY PLOT2(IMAGE,XMAX,XMIN,YMAX,YMIN)
      KPLOT2=.TRUE.
      IF (KPLOT1) GO TO 1200
      NSCL=0
      NH=5
      NSH=10
      NV=10
      NSV=10
      GO TO 200
1200      CONTINUE
      IF (.NOT.KPLOT) RETURN
      YMX=YMAX
      DH=(YMAX-YMIN)/FLOAT(NDH)
      DV=(XMAX-XMIN)/FLOAT(NDV)
      DO 1300 I=1,NVP
1300      ABNOS(I)=(XMIN+FLOAT((I-1)*NSV)*DV)*FSX
```

```
      DO 1400 I=1,NIMG
1400      IMAGE(I)=BL
      DO 1800 I=1,NDHP
      I2=I*NDVP
      I1=I2-NDV
      KNHOR=MOD(I-1,NSH).NE.0
      IF (KNHOR) GO TO 1600
      DO 1500 J=I1,I2
1500      IMAGE(J)=HC
1600      CONTINUE
      DO 1800 J=I1,I2,NSV
      IF (KNHOR) GO TO 1700
      IMAGE(J)=NC
      GO TO 1800
1700      IMAGE(J)=VC
1800      CONTINUE
      XMIN1=XMIN-DV/2.
      YMIN1=YMIN-DH/2.
      RETURN
C
      ENTRY PLOT3(IMAGE,CH,X,Y,N3)
      IF (KPLOT2) GO TO 2100
1900      WRITE (60,2000)
2000      FORMAT (T5,'PLOT2 MUST BE CALLED')
2100      CONTINUE
      IF (.NOT.KPLOT) RETURN
      IF (N3.GT.0) GO TO 2300
      KPLOT=.FALSE.
      WRITE (60,2200)
2200      FORMAT (T5,'PLOT3, ARG4 <.OR.= 0')
      RETURN
2300      DO 3000 I=1,N3
      IF (DV) 2500,2400,2500
2400      DUM1=0
      GO TO 2600
2500      CONTINUE
      DUM1=(X(I)-XMIN1)/DV
2600      IF (DH) 2800,2700,2800
2700      DUM2=0
      GO TO 2900
2800      CONTINUE
      DUM2=(Y(I)-YMIN1)/DH
2900      CONTINUE
      IF (DUM1.LT.0..OR.DUM2.LT.0.) GO TO 3000
      IF (DUM1.GE.NDVP.OR.DUM2.GE.NDHP) GO TO 3000
      NX=1+INT(DUM1)
      NY=1+INT(DUM2)
      J=(NDHP-NY)*NDVP+NX
      IMAGE(J)=CH
3000      CONTINUE
      RETURN
C
      ENTRY PLOT4(NL,LABEL,IMAGE)
      ENTRY FPLOT4(NL,LABEL,IMAGE)
```

```
      IF (.NOT.KPLOT) RETURN
      IF (.NOT.KPLOT2) GO TO 1900
      DO 3200 I=1,NDHP
      IF (I.EQ.NDHP.AND.KBOTGL) GO TO 3200
      WL=BL
      IF (I.LE.NL) WL=LABEL(I)
      I2=I*NDVP
      I1=I2-NDV
      IF (MOD(I-1,NSH).EQ.0.AND..NOT.KORD) GO TO 3100
      WRITE (3,FOX2) WL,(IMAGE(J),J=I1,I2)
      GO TO 3200
3100      CONTINUE
      ORDNO=(YMX-FLOAT(I-1)*DH)*FSY
      WRITE (3,FOX1) WL,ORDNO,(IMAGE(J),J=I1,I2)
3200      CONTINUE
      IF (KABSC) GO TO 3300
      WRITE (3,FOX3) (ABNOS(J),J=1,NVP)
3300      RETURN
C
      ENTRY OMIT(LSW)
      KABSC=MOD(LSW,2).EQ.1
      KORD=MOD(LSW,4).GE.2
      KBOTGL=LSW.GE.4
      RETURN
3400      FORMAT (19A1)
3500      FORMAT (15A1)
      END
      SUBROUTINE UNIQUE(YC,I,J,JDFLAG)
C
-----------------------------------------------------------------
C
C         UNIQUE......
C
C     THE SUBROUTINE  UNIQUE SERVES AS A "TRAFFIC COP" TO DIRECT
THE
C           FLOW OF THE PROGRAM TO THE RIGHT SUBROUTINE FOR THE
CALCULATION
C        OF YC AND DC(I) FOR THE PARTICULAR "AD HOC" CONSTRAINT AS
C         PERCEIVED AND PROGRAMMED BY THE USER. A DUMMY EXAMPLE IS
C         GIVEN.  HOWEVER, THE PROGRAM, AS SUPPLIED, WILL PRINT AN
C         ERROR MESSAGE AND TERMINATE.  WHEN USED, THE SUBROUTINES
C         "LOG_R", "LOG_FO2", ETC WOULD BE SUPPLIED
C         AND THE "C" ON THE LINES BELOW WOULD HAVE BEEN REMOVED.
C
C
-----------------------------------------------------------------
      IMPLICIT REAL*8(A-H,O-Z)
C
-----------------------------------------------------------------
C
C       PARAMETERS STATEMENTS.  THESE HAVE BEEN ENTERED IN EACH
ROUTINE
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C         DIMENSIONS WHERE STORAGE SPACE IS SHORT.  THESE CHANGES
```

```
MAY BE
C        MADE TO COVER INCREASES IN THE NUMBER OF PARAMETERS PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
----------------------------------------------------------------
      DIMENSION COEF(IP4,IP3),TINV(IP4,IP3,IP10),NPHASE(IP3),
               1
IKOUNT(IP3),IGO(IP3),ISTATE(IP4,IP3),INSTAT(IP4,IP3),
     2        INVPH(IP4,IP3,IP11),INVSC(IP4,IP3),ISPECL(IP4,IP3),
     3          IPHASE(IP4,IP3),NINVER(IP4,IP3)
      COMMON /EARTH/ COEF,TINV,NPHASE,IKOUNT,IGO,ISTATE,INSTAT,
     1               INVPH,INVSC,ISPECL,IPHASE,NINVER,NSETS,LISTP
C     IGOES=IGO(J)-107
C     GO TO (8,9,10,11,12,13,14,15,16,17,18,19,20,9999),
C    1         IGOES
C   8 CONTINUE
C     CALL LOG_R(YC,I,J,JDFLAG)
C     RETURN
C   9 CONTINUE
C     CALL LOG_FO2(YC,I,J,JDFLAG)
C     RETURN
C  10 CONTINUE
C     CALL DELTA_E(YC,I,J,JDFLAG)
C     RETURN
C  11 CONTINUE
C     CALL LOG_O2IW(YC,I,J,JDFLAG)
C     RETURN
C  12 CONTINUE
C     CALL EMF_O2IW(YC,I,J,JDFLAG)
C     RETURN
C  13 CONTINUE
C     CALL EMF_O2WM(YC,I,J,JDFLAG)
C     RETURN
C  14 CONTINUE
C     CALL EMF_O2IM(YC,I,J,JDFLAG)
C     RETURN
C  15 CONTINUE
C     CALL LOG_O2WM(YC,I,J,JDFLAG)
C     RETURN
C  16 CONTINUE
C     CALL LOG_O2X(YC,I,J,JDFLAG)
C     RETURN
C  17 CONTINUE
C     CALL LOG_O2IM(YC,I,J,JDFLAG)
C     RETURN
C  18 CONTINUE
C     CALL COMP_X(YC,I,J,JDFLAG)
C     RETURN
C  19 CONTINUE
C     CALL EMF_BRK(YC,I,J,JDFLAG)
```

```
C     RETURN
C  20 CONTINUE
C     CALL VOL_FEO(YC,I,J,JDFLAG)
C     RETURN
C9999 CONTINUE
      WRITE (60,60) J,J,IGO(J)
      STOP
c  DG.    fORMAT REFORMATTED
   60 FORMAT (6H0YOUR ,I3,39H-TH DATA SET CALLED UNIQUE FROM EAFW
. ,
     1 /,5H IGO(,I2,17H) HAS A VALUE OF ,I6,
     2    38H BUT UNIQUE IS CURRENTLY UNPROGRAMMED.      )
      END
      SUBROUTINE ERRORS
C
-----------------------------------------------------------------
C     CALL SYSTEM ERROR-TRAPS FOR:
C         -- FLOATING UNDERFLOW IN MATH LIBRARY.
C
-----------------------------------------------------------------
      CALL UNDER0(.TRUE.)
      RETURN
      END
      SUBROUTINE TIMELY(DATTIM)
C
-----------------------------------------------------------------
C     PROGRAM PRESENTLY SET TO USE "DATE_TIME" INTERFACE ROUTINES
FROM
C       THE IBM DISC OPERATING SYSTEM (DOS).
C
-----------------------------------------------------------------
      CHARACTER*1 ADATE,BLANK
      CHARACTER*8 DCHAR
      CHARACTER*11 TCHAR
      CHARACTER*23 DATTIM,DT
      DIMENSION ADATE(23)
      EQUIVALENCE (DT,ADATE(1))
      EQUIVALENCE (ADATE(1),DCHAR)
      EQUIVALENCE (ADATE(10),TCHAR)
      DATA BLANK/' '/
      ADATE(9)=BLANK
      ADATE(21)=BLANK
      ADATE(22)=BLANK
      ADATE(23)=BLANK
      CALL DATE(DCHAR)
      CALL TIME(TCHAR)
      DATTIM=DT
      RETURN
      END
      FUNCTION DIE(T)
      IMPLICIT REAL*8(A-H,O-Z)
C
-----------------------------------------------------------------
C
```

```
C      PARAMETERS  STATEMENTS.   THESE  HAVE  BEEN  ENTERED  IN  EACH
ROUTINE
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C         DIMENSIONS  WHERE  STORAGE  SPACE  IS  SHORT.   THESE  CHANGES
MAY BE
C         MADE  TO  COVER  INCREASES  IN  THE  NUMBER  OF  PARAMETERS  PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
----------------------------------------------------------------
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
C
----------------------------------------------------------------
C     COMMON BLOCKS
C
----------------------------------------------------------------
                    C   O   M   M   O   N      /   W   A   T   E   R   /
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1               STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      DIE=DEXP(FN(T)+T/THETA)/DIEO
      RETURN
      END
      FUNCTION FN(T)
      IMPLICIT REAL*8(A-H,O-Z)
C
----------------------------------------------------------------
C
C      PARAMETERS  STATEMENTS.   THESE  HAVE  BEEN  ENTERED  IN  EACH
ROUTINE
C        IN THIS PROGRAM.  CHANGING THEM WILL CHANGE THE CRITICAL
C         DIMENSIONS  WHERE  STORAGE  SPACE  IS  SHORT.   THESE  CHANGES
MAY BE
C         MADE  TO  COVER  INCREASES  IN  THE  NUMBER  OF  PARAMETERS  PER
PHASE,
C        ALSO.
C
      INCLUDE PARAM.FOR
C
C
----------------------------------------------------------------
      DIMENSION SCINV(2),STCOEF(10),TK(19,2),NSCALE(5)
C
----------------------------------------------------------------
C     COMMON BLOCKS
C
----------------------------------------------------------------
                    C   O   M   M   O   N      /   W   A   T   E   R   /
ZERO,ONE,TWO,THREE,FOUR,SIX,R,F,A,SCINV,TREF,PREF,
     1               STCOEF,DIEO,ADIE,BDIE,THETA,TK,NL,NSCALE
      FN=DEXP(BDIE+ADIE*T)
      RETURN
      END
```