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THERMODYNAMIC DATA FOR IRON
FROM 200 TO 3000 K AND FROM 0 TO 200 KBAR

(A Preliminary Report to the
CODATA Task Group on Chemical Thermodynamic Tables)

by

John L. Haas, Jr. and Malcolm W. Chase, Jr.

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John L. Haas, Jr.
U.S. Geological Survey
National Center, Mail Stop 959
Reston, Virginia 22092, U.S.A.

and

Malcolm W. Chase, Jr.
National Institute for Standards and Technology
Office of Standard Reference Data
Gaithersburg, Maryland 20899, U.S.A.

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NOTICE

This report has been supplied to the CODATA Task Group on Chemical Thermodynamic Tables for use in formulating an evaluation of the properties of iron. The report is preliminary and should not be used as the basis for other research without contacting members of the Task Group as to the final disposition.

INTRODUCTION

There have been many attempts to evaluate the thermodynamic properties of iron. Some amount to simple smoothing of experimental data for one or more phases over limited ranges of temperature. Others, such as the work of Fernandez Guillermet and Gustafson (1985), pick key values and attempt to fit those data closely. In the fitting, model equations and thermodynamic relations were used to smooth over the pressure and temperature conditions where data were either unreliable or unavailable.

This study used a set of experimental data, three empirical functions, and thermodynamic relations among the properties to make a more complete evaluation of the properties of the three solid polymorphs, Fe(bcc), Fe(fcc), and Fe(hcp) and the liquid phase, Fe(liq). (Structural notation is used for the solids because the notation contains explicit information whereas the parallel notation, Fe(alpha), Fe(gamma), and Fe(epsilon) does not.) Empirical functions are used as the basis for the descriptions of the molar heat capacity, the cubic expansivity coefficient and the isothermal bulk modulus. These functions will be discussed in a later section in this report.

Fernandez Guillermet and Gustafson (1985) achieved a reasonable description of the thermodynamic properties of iron through the use of model equations fitting both the volumetric and thermal functions for the three solid polymorphs of iron and for liquid iron. In this study, their results are being refined to achieve:

1. a better description of the heat capacity for Fe(bcc) near 298.15 K and near the second-order magnetic anomaly at 1043.2 K,

2. an improvement in the volume functions to agree better with the observed anomaly at 1043.2 K, and
3. an improvement in the fit of the molar volumes both at high temperatures and at high pressures.

None of the successes achieved by Fernandez-Guillermet and Gustafson (1985) were sacrificed to achieve these improvements.

NOMENCLATURE AND PHYSICAL CONSTANTS

The nomenclature for physical and thermodynamic properties and the symbols used in this report are consistent with the recommended usage of the International Union for Pure and Applied Chemistry (Mills and others, 1988). However, the units used in this report are those appropriate for the optimization program that was used to perform this evaluation. (Refer to section on method, below.)

The values for the fundamental constants are as recommended by the CODATA Task Group on Fundamental Constants (Cohen and Taylor, 1986). They are as follows:

Avogadro constant	$L = 6.0221367 \times 10^{23}$ mol^{-1}
Faraday constant	$F = 96485.309$ C mol^{-1}
gas constant	$R = 8.314510$ J K^{-1} mol^{-1}

In addition, the thermochemical calorie is defined as follows:

$$1 \text{ cal(th)} = 4.184 \text{ J, exactly.}$$

The relative atomic weight of iron is 55.487 g mol^{-1} as recommended by the IUPAC Commission on Atomic Weights and Isotopic Abundances (Mills and others, 1988).

The reference temperature and the reference pressure for the equations used here are 298.15 K and 1 bar (= 10^5 Pa).

The following fixed temperature points were used for the transitions indicated:

TRANSITION	TEMPERATURE	SOURCE
T_C, Fe(bcc)	1043.2 K	Kollie (1969)
T[Fe(bcc)=Fe(fcc)]	1184	Chase and others (1985)
T[Fe(fcc)=Fe(bcc)]	1665	Chase and others (1985)
T[Fe(bcc)=Fe(liq)]	1809	Chase and others (1985)

No adjustments were made for most data. Correcting data that did not already fit these fixed points is very difficult. The Curie temperature of Fe(bcc) is sensitive both to temperature measurement errors and to the amount and types of impurities. Many studies reported the Fe(bcc)-Fe(fcc) transition as 1184±1 K but T_C would be as much as 10 to 15 kelvins lower than the accepted value of 1043.2 K. The studies used here required minimal changes to agree with the above fixed points.

The pressure scale used in this study is consistent with the ruby pressure standard, calibrated against the elements silver and copper (Mao and others, 1986).

METHOD

The optimization method of Haas and Fisher (1976) was modified and used for this evaluation. The method evaluates and fits a series of thermodynamically related functions to the observed data for a defined chemical system. The modifications include:

1. expanding the heat capacity function to include additional terms,

2. introducing the Inden function for Cp anomalies associated with second-order magnetic disordering (Inden, 1981),
3. revising completely the equation for volume to incorporate the first-order Murnaghan equation of state* and to follow more closely the earlier evaluation by Fernandez Guillermet and Gustafson (1985),
4. introducing a correction in the volume function so that the anomaly in volume, associated with magnetic disordering, can also be included,
5. adding provisions to fit the cubic expansion coefficient and both the isothermal and isentropic compressibilities, and
6. adding a provision to fit the critical temperature, T_C, as a function of pressure.

One other modification of the method proposed by Haas and Fisher (1976) was incorporated. The reference state for the elements at the reference pressure was changed from $\Delta_f G°(298.15 \text{ K}, 1 \text{ atm}) = 0$ to $\Delta_f H°(298.15 \text{ K}, 1 \text{ bar}) = 0$. This change brings the optimization program into agreement with common usage where enthalpy is the reference property and where the bar (= 10^5 Pa) is the reference pressure.

Fitting of phase equilibria and molar volumes at high pressures was accomplished by adding the pressure of the experiment and the reference pressure, if any, as the third and fourth independent variables, respectively.

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* The first-order Murnaghan equation (Murnaghan, 1944) is as follows:

$$V(T,P)/V(T,Pr) = (1 + n\, P/K_T)^{-1/n},$$

where K_T is the isothermal bulk modulus at T and P and n is the first derivative of the isothermal bulk modulus with respect to pressure, P.

The temperature of the experiment and a reference temperature, if any, are the first and second independent variables, respectively.

To achieve the optimization of the functions, each observation was weighted equivalent to the reciprocal of the square of the author's stated (or implied) precision. There were minor exceptions where the author provided a precision that was not supported by the observations. The precision was used because an estimate of the accuracy is not available until the evaluation is completed. Weighting of the data is important and is necessary for a useable optimization because the data varies by as much as 10 orders in magnitude. For example $\Delta_{fus}H°$ for Fe(bcc) = Fe(liq) at 1809 K is 13,850 J/mol and the isentropic bulk modulus of Fe(bcc) is approximately 0.6×10^{-6} bar^{-1}.

DATA

The results of this evaluation were obtained by considering experimental data and theoretical constraints only. The results from commonly available evaluations were included for comparison only. The data included the following measured properties:

1. heat capacity, $Cp°(T,Pr)$,
2. entropy, $S°(298.15K,Pr)$,
3. incremental enthalpies, $H°(T,Pr)-H°(Tr,Pr)$,
4. enthalpy of inversion, $\Delta_i H°(T,Pr)$,
5. phase equilibria as a function of temperature and pressure, $\Delta_i G(T,P) = 0$,
6. molar volumes, $V_m(T,P)$,
7. crystallographic lattice constants, $a_0(T,P)$ [or $a_0(T,P)$ and $c_0(T,P)$ for Fe(hcp)],

8. reduced volumes, V(T,P)/V(Tr,Pr),
9. relative volumes, [V(T,P)-V(Tr,Pr)]/V(Tr,Pr),
10. cubic expansion coefficients, $\alpha(T,P)$,
11. apparent cubic expansion coefficients,
    [V(T,P)-V(Tr,Pr)]/[V(Tr,Pr)(T-Tr)],
12. isothermal compressibilities, $\kappa_T(T,P)$,
13. apparent isothermal compressibilities,
    [V(T,P)-V(Tr,Pr)]/[V(Tr,Pr)(P-Pr)],
14. isothermal bulk moduli, $K_T(T,P)$,
15. isentropic compressibility, $\kappa_S(T,P)$,
16. isentropic bulk moduli, $K_S(T,P)$,
17. slope of a phase inversion, dP/dT, at P = 0 bar, and
18. critical temperature, T_c, as a function of pressure.

The data do not restrict the trend of the calculated heat capacities of the solids above their stability fields. To prevent anomalous extrapolations of the polynomials for the heat capacities of the solids, use was made of the Petit-Dulong limit. The limiting equation is shown below,

$$\lim_{T\to\infty} C_p = 3\ n\ R + \frac{\alpha^2\ V\ T}{10\ \kappa_T} \qquad 1.$$

where n is the number of atoms in the formula unit, R is the gas constant, α is the cubic expansion coefficient, V is the molar volume, and κ_T is the isothermal compressibility. Absolute values could not be used because the electronic contribution to the heat capacity could not be estimated independently at temperatures greater than 2000 K. Differences in the heat capacities were calculated at 500 kelvin intervals between 2000 and 4000 K. These differences were included as part of the fitted data set to insure that the slopes were qualitatively in agreement with them. Because electronic contributions would add to the heat capacity in this temperature region, the differences were considered minimum values to be achieved in the fitting.

In addition, the theoretical estimates of the total contribution to entropy, S(T), from the disordering of the magnetic structure were included.

RESULTS

INTRODUCTION

The results of the fit will be discussed by property. The order of the discussion will be as follows:

Heat capacity and incremental enthalpy
Entropy
Enthalpy
Gibbs energy of inversion at 1 bar
Volume of the solids
Volume of the liquid
Cubic expansion coefficient
Isothermal compressibility and isothermal bulk modulus
Isentropic compressibility and isentropic bulk modulus
The critical temperature
Phase equilibria at elevated pressures

The equations will be given with each discussion. Table 1 contains the constants for use in the equations.

HEAT CAPACITY AND INCREMENTAL ENTHALPY

The fitting functions for the heat capacity and the incremental enthalpy are given by equations 2 through 7.

$$C_p° = a_1 T^{-3} + a_2 T^{-2} + a_3 T^{-1} + a_4 T^{-.5} + a_5 + a_6 T + a_7 T^2 + a_8 T^3 + C_p(M,T) \qquad 2.$$

$C_p(M,T)$ is the contribution to the heat capacity that is caused by the disordering of the magnetic structure of Fe(bcc) and Fe(fcc). The contribution is calculated using the following functions for T less than or equal to and for T greater than T_c, respectively. The term tau is the ratio of T to T_c.

$$C_p(M,T<T_c) = a_{13} \sum_{k=1}^{n} \frac{\tau^{[j'(2k-1)]}}{2k-1} \qquad 3.$$

and

$$C_p(M,T>T_c) = a_{14} \sum_{k=1}^{n} \frac{\tau^{[j''(2k-1)]}}{2k-1} \qquad 4.$$

$$\begin{aligned} H°(T,i)-H°(Tr,j) = {} & -0.5\ a_{1,i}\ T^{-2} - a_{2,i}\ T^{-1} + a_{3,i}\ \ln(T) + 2\ a_{4,i}\ T^{.5} + a_{5,i}\ T \\ & + 0.5\ a_{6,i}\ T^{2} + a_{7,i}\ T^{3}/3 + a_{8,i}\ T^{4}/4 + a_{9,i} + H(M,i,T) \\ & + 0.5\ a_{1,j}\ Tr^{-2} + a_{2,j}\ Tr^{-1} - a_{3,j}\ \ln(Tr) - 2\ a_{4,i}\ Tr^{.5} - a_{5,i}\ Tr \\ & - 0.5\ a_{6,j}\ Tr^{2} - a_{7,j}\ Tr^{3}/3 - a_{8,j}\ Tr^{4}/4 - a_{9,j} - H(M,j,Tr) \qquad 5. \end{aligned}$$

In the last function, Tr is the reference temperature for the observation. The subscripts i and j refer to the phases present at T and Tr, respectively. The phases may or may not be the same. For example, for Fe(bcc), the phases at T and Tr are the same but for the others, the phase at Tr is always Fe(bcc).

H(M,i or j,T) is the contribution to the heat capacity that is caused by the disordering of the magnetic spin structure of Fe(bcc) and Fe(fcc). The contribution is calculated using the following functions for T less than or equal to and for T greater than T_c, respectively.

$$H(M,T<T_c) = T_c\ a_{13} \sum_{k=1}^{n} \frac{\tau^{[j'(2k-1)+1]}}{(2k-1)(j'(2k-1)+1)} \qquad 6.$$

and

$$H(M,T>T_C) = T_C\, a_{14} \sum_{k=1}^{n} \frac{\tau^{[j''(2k-1)+1]}}{(2k-1)(j''(2k-1)+1)}$$

$$+ a_{13} \sum_{k=1}^{n} \frac{T_c}{(2k-1)[j'(2k-1)+1]} - a_{14} \sum_{k=1}^{n} \frac{T_c}{(2k-1)[j''(2k-1)+1]} \qquad 7.$$

The heat capacities and the incremental enthalpies for the solid polymorphs from 200 to 3000 K and for the liquid from 1000 to 3000 K were calculated using these functions and the constants given in Table 1. These smoothed values are given in Tables 2 and 3, respectively. Figure 1 is a plot of the calculated heat capacities between 200 and 2500 K. Figure 2 contains the same data but the properties of the metastable phases have been deleted. Figure 3 through 26 give the plots of the calculated heat capacities and the data contained in the sources indicated on the figures.

Figure 27 shows the calculated incremental enthalpies for the three solids and the liquid to 2500 K. Figures 28 through 38 give the plots of the calculated incremental enthalpies and the data contained in the sources cited.

Data from Anderson and Hultgren (1962), Dench and Kubachewski (1963), Eucken and Werth (1930), Fernandez Guillermet and Gustafson (1985), Ferrier and Olette (1962), Kelley (1943), Kollie and others (1969), Morris and others (1966), Olette and Ferrier (1958), Rogez and LeCoze (1980), Stepakoff and Kaufman (1968), Tsuchiya and others (1971), Vollmer and others (1966), and Zuitoff (1938) were used in this evaluation. The data were given weight equivalent to the reciprocal of the square of the author's stated precision.

From the compilation by Fernandez Guillermet and Gustafson (1985), only the smoothed estimated values for Fe(hcp) were used. The precision was set at five percent. This was done to contain in the fitted data set some guide for the fitting of the heat capacity function for Fe(hcp) at elevated temperatures. The resulting weight was sufficiently low that it would not force the fit from this evaluation to be the same as that obtained by Fernandez Guillermet and Gustafson.

The following paragraphs are a study-by-study review of the results as compared to the sources of data or to the cited compilation. The comparison with compilations is included for the readers' benefit so that they may recognize how this study differs from data that they may be using.

Austin (1932). Figure 3 shows Austin's evaluated results and the fitted line from this study. Agreement, particularly at lower temperatures, is reasonable for Fe(bcc) but Austin's estimated values for Fe(fcc) are high. The heat capacity of Fe(fcc) was estimated by Austin by averaging values derived from a Debye function and the Kopp-Neuman rule. (See also Eucken and Werth, 1930.) The data were given zero weight in the fitting process.

Awbery and Griffith (1940). Figure 4 shows the smoothed heat capacities of Awbery and Griffith and the fitted curves. Agreement below T_C is consistent with the precision of the data. However, above T_C the fitted functions are significantly higher than the Awbery and Griffith's data. The data were given zero weight.

Bendick and Pepperhoff (1982). The authors measured the heat capacity of the stable phase from 300 to approximately 1720 K. Their experimental data and theory were used to derive the smoothed heat capacities of Fe(bcc) and Fe(fcc) as shown on Figure 5. The agreement between this evaluation and the work of Bendick and Pepperhoff is not good. An attempt to base the evaluation of C_p of Fe(bcc) and Fe(fcc) only on Bendick and Pepperhoff's study caused systematic errors in $\Delta_i H^\circ$ for the inversion of Fe(fcc) to Fe(bcc) between 1184 and 864 K. Refer to Figure 41 for an indication of the disagreement between this study and that of Bendick and Pepperhoff. In addition the P-T curve for the equilibrium "Fe(fcc) = Fe(hcp)" were not fit properly as compared to this evaluation. The data were given zero weight in the final fitting process.

Cezairlyan and McClure (1975). Use was made of a subsecond pulse heating technique to measure the heat capacity of Fe(fcc) and Fe(bcc) between 1500 and 1800 K (Figure 6). The fitted values for Fe(fcc) are in consistent with the precision of the data. The fitted function for Fe(bcc) has a lower temperature dependence than the experimental data. The data were not used in the fitting process because the anomalous slope in Fe(bcc) could not be justified by other data.

Chase and others (1985). This study is also referred to as the JANAF Thermochemical Tables. The smoothed values given in the JANAF Thermochemical Tables are plotted on Figure 7 for comparison with this evaluation (lines). Agreement is good except for the heat capacities of Fe(bcc) at temperatures above 1500 K. The data for Fe(fcc) in the JANAF Thermochemical Tables are based on a linear fit of the data within the stability range. Therefore, the properties of the metastable phase below 1184 K will also deviate in a systematic fashion from this evaluation. In this study, the heat capacity of Fe(fcc) was fit with a more complex polynomial in temperature. The JANAF data were given zero weight in this review.

Darken and Smith (1951). The review by Darken and Smith, though based on an analysis of different data is close to the results of this evaluation in most details (Figure 8). The results of the review were given zero weight.

Dench and Kubachewski (1963). Heat contents over short temperature intervals of 20 to 30 kelvin were made between 1073 and 1800 K but the results were reported as smoothed heat capacities (Figure 9). The results from this review are in agreement with the smoothed heat capacities except that the fitted values are high. The data have a stated precision of 2 percent and the fitted function is within that precision.

Desai (1986). Smoothed evaluated heat capacities from Desai's review are plotted on Figure 10 along with the fitted functions. Desai's values for Fe(bcc) above 1665 K are based on the experimental work of Cezairlyan and McClure (1975). This alone accounts for most of the differences between the two evaluations. Such high temperature dependence for the heat capacity of Fe(bcc) would make it difficult to fit the Fe(bcc) to Fe(fcc) inversion and the melting of Fe(bcc) at higher pressures. The data in the review were given zero weight because no new data were presented.

Dobrosavljevic and others (1985). A pulse heating technique was used to measure the heat capacity of iron to 1750 K. The averaged values and the fitted functions from this study are plotted on Figure 11. The averaged values are systematically higher than the fitted functions, but the precision of the experimental data is about 1 percent. The data were given zero weight in this evaluation.

Eucken and Werth (1930). The heat capacity of iron and iron-manganese alloys were measured between 16 and 200 K. From these data the heat capacity of Fe(fcc) was estimated. The data between 150 and 200 K were used in this evaluation. Figure 12 shows the data used ("+") and the fitted function.

Considered the extrapolations and the precision of the data, the agreement of the functions to the observations is acceptable.

Fernandez Guillermet and Gustafson (1985), This study is also referred to as the KTH* compilation. In almost all respects the KTH compilation and this evaluation are similar. Refer to Figures 13 and 14. The KTH evaluations used a constant heat capacity of 46 J/(mol K) for the heat capacity of the liquid. The evaluated smoothed results for Fe(bcc), Fe(fcc), and Fe(liq) from the KTH evaluation were not used in this study. As stated above, the data for Fe(hcp) were given a low weight.

Holetzko (1952; cited in Krauss, 1958). Krauss (1958) cites data from the dissertation by Holetzko (1952). They are plotted on Figure 15 along with the fitted functions. Up to T_c the fitted function for Fe(bcc) agrees well with the reported data. However, above T_c, the fitted functions are not in agreement. In part, some of the scatter is due to the inclusion of part of the enthalpy of inversion at 1184 and 1665 K in the heat capacities. The data were given zero weight.

Kelley (1943). Heat capacities were measured up to 295.1 K (Figure 16, "o"). The data between 155 and 295.1 K were used to complete this evaluation. Agreement is within the precision of the experimental data.

Klinkhardt (1927). Values from Klinkhardt's smoothed functions for Fe(bcc) and Fe(fcc) are plotted on Figure 17 along with the fitted functions for this study. Agreement of the heat capacity for Fe(bcc) is consistent with the scatter of Klinkhardt's experimental data as shown in Figure 9 of the cited reference. For Fe(fcc), the agreement is not acceptable. Klinkhardt's

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* KTH refers to the Royal Institute of Technology, Stockholm, Sweden.

experimental values above 1184 are uniformly higher than the fitted function from this study. Klinkhardt's data were given zero weight.

Kohlhaas and others (1966); Vollmer and others (1966). These related studies supplied smoothed data for the heat capacities of iron from 300 to 1860 K (Figure 18). The first report gives details around T_C and the second report gives data over the complete temperature range. The observed heat capacity for Fe(fcc) is about 1 to 2 percent lower than the fitted function. The observed heat capacity for the liquid is 43.0 J/(mol K) and is consistent with the fitted function that yields 43.2 J/(mol K) at the melting point, 1809 K. The data were given a weight consistent with the authors' stated precision of 2 percent.

Kollie and others (1969); Kollie (1969). A pulse calorimeter was used to measure the heat capacity of iron from 333 to 1478 K. Smoothed values are graphed on Figure 16 ("+") along with the fitted functions. The data were used in completing this evaluation. The fit of the function for Fe(bcc) is excellent but the data for Fe(fcc) are systematically above the fitted curve and have a different trend with temperature. This latter departure is the result of a minor disagreement among these data, incremental enthalpies to be discussed later, and the phase equilibria.

Lapp (1936; cited by Krauss, 1958). Krauss (1958) cited Lapp's data (Figure 19, "o") in his review paper. The data are systematically higher than the fitted function and were given zero weight.

Lehman (1960). Two observations are plotted on Figure 19. The data were given zero weight because they are anomalous.

Margrave (1975). Margrave, in his compilation, reported the heat capacity of Fe(liq) near the melting temperature as 46.44 J/(mol K). Refer to

Figure 19. In this evaluation, the fitted heat capacity varies from 43.19 J/(mol K) at 1809 to 43.78 J/(mol K) at 2000 and 45.87 J/(mol K) at 3000 K.

Orr and Chipman (1967). The compilation is in agreement with the evaluation of Orr and Chipman except for for the heat capacities of Fe(bcc) above 1500 K and of the liquid. Refer to Figure 20. In both cases, Orr and Chipman estimated an average heat capacity for the temperature range from the available data. For Fe(bcc) the heat capacity was adjusted to yield that "average" value and yet be consistent with the metastable extrapolation of the heat capacity above 1184 K. For the liquid, the average heat capacity was used directly. The approach in this study was to fit the data for each phase over the complete temperature range with one polynomial in T (equation 2) and a function for the anomaly (equations 3 and 4). The approach used here considered the enthalpies of inversion at 1184, 1665, and 1809 K, the molar volumes, activities of Fe in several alloys, and the univariant reactions as a function of pressure. Orr and Chipman considered the enthalpies and activities but made no attempt to include volume data and the univariant reactions at elevated pressures in their evaluation. Their results were given zero weight in this evaluation because this study was an evaluation of published data only.

Pallister (1949). Heat capacities were measured from 273 to 1523 K. Pallister's smoothed data were compared with the fitted curves from this study on Figure 21. Up to the critical temperature, the agreement is consistent with the precision of the experimental data.. Above T_C the data for both Fe(bcc) and Fe(fcc) are low and show a maximum difference near 1184 K. The data were given zero wieght.

Rogez and LeCoze (1980). Agreement with the Cp data measured by Rogez and LeCoze is satisfactory. Refer to Figure 22. The precision of the measurements was reported as 2.5 percent. The data were given a low weight in this evaluation consistent with the stated precision.

Stepakoff and Kaufman (1968). The heat capacity of Fe(bcc) and iron-ruthenium alloys from 36 to 100 percent Ru were measured. The data for Fe(bcc) are shown on Figure 23 and were used in completing this evaluation. The agreement between the observed and calculated values is less than the experimental precision.

The heat capacity of Fe(hcp) was obtained by Stepakoff and Kaufman from linear extrapolations of the data for the alloys and for pure ruthenium. The extrapolating curves were reported to be linear functions of mole percent of Fe to within 1 percent. These data were used in this evaluation as part of the fitted data. Refer to Figure 12 ("o") for a comparison of the fitted function with the "observed" values of Stepakoff and Kaufman.

Tsuchiya and others (1971). Heat capacities of a series of iron-nickel and iron-manganese alloys having the face-centered cubic structure were measured between 300 and 900 K. Tsuchiya and coworkers combined these data with the research of Eucken and Werth (1930) to estimate the heat capacity of Fe(fcc) from 0 to 1800 K. In this study the data between 300 and 900 K were used as part of the fitted set for the heat capacity of Fe(fcc). Figure 24 shows the comparison.

Valentiner (1958). Molar heat capacities were measured between room temperature and the critical temperature. The data are anomalously high and were given zero weight. Refer to Figure 25.

Wallace and others (1960). The heat capacity of iron from 298 to 1323 K using a dynamic pulse heating method was measured (Figure 26). The data were not used in this evaluation. The departure between T_C and 1184 K indicates that the data of Wallace and others are not consistent with the data for the reaction Fe(fcc) = Fe(bcc) at temperatures below 1184 K.

Anderson and Hultgren (1962). Incremental enthalpies were measured over the temperature range 298 to 1433 K (Figure 28). The data were found to be totally consistent with all other parts of the data set for iron and were used. The largest difference between the observed and the fitted values was 315 J/mol at 1031 K. The average difference was 90 J/mol, a value well within the precision of the data.

Esser and Baerlecken (1941). The incremental enthalpies of electrolytic iron were measured to 1100 K. Refer to Figure 29. The fitted function for the incremental enthalpies is about 1 percent lower than their data from "run 2" and more than 2 percent lower than their "run 1". Esser and Baerlecken used the data from "run 2" to derive the smoothed data for iron.

Jaeger and others (1938). Incremental enthalpies were measured between 273 and 1470 K. The data are anomalously high and were given zero weight. Refer to Figure 30.

Morris and others (1966). A diphenyl ether calorimeter was used to measure the incremental enthalpies between 1725 and 1875 K (Figure 31). The data were used in this evaluation. The largest difference between the observed and fitted values was 500 J/mol at 1862 K. Just fitting the incremental enthalpies for the liquid with a function "a + bT" yielded an average heat capacity (=b) for the liquid of 39.3 J/(mol K). In this evaluation the heat capacity varied from 43.2 J/(mol K) at 1809 K to 43.8 J/(mol K) at 2000 K.

Oberhoffer and Grosse (1927). Incremental enthalpies were measured between 273 and 1870 K. The data are anomalously high and were given zero weight. Refer to Figure 32. Just fitting the incremental enthalpies for the liquid with a function "a + bT" yielded an average heat capacity (=b) for the liquid of 34.6 J/(mol K). In this evaluation the heat capacity varied from 43.2 J/(mol K) at 1809 K to 43.8 J/(mol K) at 2000 K.

Olette and Ferrier (1958), Ferrier and Olette (1962). The data were measured by an adiabatic drop calorimeter between 1193 and 2213 K. Refer to Figure 33. The data were found to be consistent with the other data accepted in this compilation and were used. The largest differences between the observed and calculated values are 554 J/mol at 1663 for Fe(fcc), 275 J/mol at 1745 K for Fe(bcc), and 879 J/mol at 2066 for Fe(liq). In the same order, the average errors are 300, 110, and 700 J/mol, respectively. The data for Fe(liq) were given a precision of 600 J/mol because error in addition to the experimental error was introduced during the scaling of the values from the figure in the paper by Ferrier and Olette (1962). Just fitting the incremental enthalpies for the liquid with a function "a + bT" yielded an average heat capacity (=b) for the liquid of 47.0 J/(mol K). In this evaluation the heat capacity varied from 43.2 J/(mol K) at 1809 K to 43.8 J/(mol K) at 2000 K.

Pattison and Willows (1956). Incremental enthalpies were measured between 1280 and 1920 K. The data are anomalously high and were given zero weight. Refer to Figure 34. Just fitting the incremental enthalpies for the liquid with a function "a + bT" yielded an average heat capacity (=b) for the liquid of 34.6 J/(mol K). In this evaluation the heat capacity varied from 43.2 J/(mol K) at 1809 K to 43.8 J/(mol K) at 2000 K.

Treverton and Margrave (1971). A levitation calorimeter was used to measure incremental enthalpies of the liquid from 1804 to 2142 K. The data, graphed on Figure 35, were found to be consistent with the other accepted data and were used. The largest difference was 740 J/mol at 2137 K. The average difference was 480 J/mol, well within the precision of the data. Just fitting the incremental enthalpies for the liquid with a function "a + bT" yielded an average heat capacity (=b) for the liquid of 43.0 J/(mol K). In this evaluation the heat capacity varied from 43.2 J/(mol K) at 1809 K to 43.8 J/(mol K) at 2000 K.

Umino (1926,1929). Incremental enthalpies were measured between 273 and 1900 K. The data are anomalously high and were given zero weight. Refer to Figure 36. Just fitting the incremental enthalpies for the liquid from Umino (1959) with a function "a + bT" yielded an average heat capacity (=b) for the liquid of 47.6 J/(mol K). In this evaluation the heat capacity varied from 43.2 J/(mol K) at 1809 K to 43.8 J/(mol K) at 2000 K.

Wust and others (1919). Incremental enthalpies were measured between 273 and 1873 K. The data are anomalously high and were given zero weight. Refer to Figure 37. Just fitting the incremental enthalpies for the liquid with a function "a + bT" yielded an average heat capacity (=b) for the liquid of 36.3 J/(mol K). In this evaluation the heat capacity varied from 43.2 J/(mol K) at 1809 K to 43.8 J/(mol K) at 2000 K.

Zuitoff (1938). Incremental enthalpies were measured between 298 and 1773 K (Figure 38). The data were used in this evaluation with the exception of the 4 values above 1665 K. The average difference was 70 J/mol. The largest difference was 207 J/mol at 1253 K.

ENTROPY

Table 4 gives the entropy, $S°(T)$ for the three solids from 200 to 3000 K and for the liquid from 1000 to 3000 K. The fitting equations are as follows:

$$S°(T) = -a_1/(3\ T^3) - a_2/(2\ T^2) - a_3/T - 2\ a_4/T^{.5} + a_5 \ln(T)$$

$$+ a_6\ T + a_7\ T^2/2 + a_8\ T^3/3 + a_{10} + S(M) \qquad 8.$$

where a_1 through a_8 are the same constants as given in the Cp function, a_{10} is the constant of integration, and $S(M)$ is the integral for $Cp(M)$.

$$S(M,\ T<T_c) = a_{13} \sum_{k=1}^{n} \frac{\tau^{[j'(2k-1)]}}{j'(2k-1)^2} \qquad 9.$$

$$S(M,\ T>T_c) = a_{14} \sum_{k=1}^{n} \frac{\tau^{[j''(2k-1)]}}{j''(2k-1)^2}$$

$$+ \ a_{13} \sum_{k=1}^{n} \frac{1}{j'(2k-1)^2} \ - \ a_{14} \sum_{k=1}^{n} \frac{1}{j''(2k-1)^2} \qquad 10.$$

In this evaluation, only three values from the literature were used as part of the fitted data. The JANAF Thermochemical Tables give S°(298.15 K,1 bar) = 27.319 J/(mol K). This is based on an earlier critical review of the available data from 0 to 400 K by one of the authors (MWC). In this review, the JANAF value was fit exactly. All other entropies as given on Table 4 were derived from the fitted thermal functions and the phase equilibria.

Hofmann and others (1956) calculated a value of 9.205 J/(mol K) for the total entropy contribution from the magnetic disordering. Chuang and others (1985) calculated a total entropy contribution as 9.324 J/(mol K). The fitted value from this optimization is 9.318 J/(mol K) in agreement with the estimate by Chuang and others (1985).

ENTHALPY

Table 5 supplies the enthalpies of inversion among the three solids from 200 to 3000 K and between the solids and the liquid from 1000 to 3000 K. These values are the results of the complete fit of the data set. The fitting equation for the enthalpy of a phase relative to H°(bcc)=0 at 298.15 K and 1 bar is as follows:

$$H°(T,i)-H°(298,Fe(bcc)) = -0.5\ a_1\ T^{-2} - a_2\ T^{-1} + a_3\ \ln(T) + 2\ a_4\ T^{-.5}$$

$$+ a_5\ T + a_6\ T^2/2 + a_7\ T^3/3 + a_8\ T^4/4 + a_9 + H(M) \qquad 11.$$

where a_1 through a_8 are the same constants as given in the heat capacity function, a_9 is the constant of integration, and H(M) is the integral of Cp(M). H(M) is calculated from the following equations.

$$H(M,T<T_C) = T_C\ a_{13} \sum_{k=1}^{n} \frac{\tau^{[j'(2k-1)+1]}}{(2k-1)(j'(2k-1)+1)} \qquad 12.$$

and

$$H(M,T>T_C) = T_C\ a_{14} \sum_{k=1}^{n} \frac{\tau^{[j''(2k-1)+1]}}{(2k-1)(j''(2k-1)+1)}$$

$$+\ a_{13} \sum_{k=1}^{n} \frac{T_C}{(2k-1)[j'(2k-1)+1]} - a_{14} \sum_{k=1}^{n} \frac{T_C}{(2k-1)[j''(2k-1)+1]} \qquad 13.$$

Table 6 gives a comparison of the optimized results and the published data. Only the data flagged with an asterisk (*) were explicitly contained in the fitted set. Other data were either given zero weight or were implicit in the incremental enthalpies described above.

GIBBS ENERGY DIFFERENCES AT 1 BAR

Table 7 gives the Gibbs energy differences among the three solids from 200 to 3000 K and between the solids and the liquid between 1000 and 3000 K. The fitting equation for the Gibbs energy of a phase relative to H°(bcc)=0 at

298.15 K and 1 bar is as follows:

$$G°(T,i)-H°(298,Fe(bcc)) = - a_1/(6\ T^2) - a_2/(2\ T) + a_3(1+\ln(T)) + 4\ a_4\ T^{.5}$$
$$+ a_5\ (T-T\ \ln(T)) - a_6\ T^2/2 - a_7\ T^3/6 - a_8\ T^4/12$$
$$+ a_9 - a_{10}\ T + G(M) \qquad 14.$$

where a_1 through a_8 are the same constants as in the heat capacity equation, a_9 and a_{10} are constants of integration for enthalpy and entropy, respectively, and G(M) is the contribution to the Gibbs energy from the disordering of the magnetic structure. G(M) is calculated using the following relation:

$$G(M) = H(M) - T\ S(M) \qquad 15.$$

Figure 39 is a plot of the Gibbs energies of all the phases relative to the Gibbs energy of Fe(bcc) For the temperature ranges indicated, the order of stability is as follows:

TEMPERATURE RANGE (K)	STABILITY SEQUENCE						
<331	Fe(bcc)	>	Fe(hcp)	>	Fe(fcc)	>	Fe(liq)
331-1184	Fe(bcc)	>	Fe(fcc)	>	Fe(hcp)	>	Fe(liq)
1184-1307	Fe(fcc)	>	Fe(bcc)	>	Fe(hcp)	>	Fe(liq)
1307-1665	Fe(fcc)	>	Fe(bcc)	>	Fe(liq)	>	Fe(hcp)
1665-1798	Fe(bcc)	>	Fe(fcc)	>	Fe(liq)	>	Fe(hcp)
1798-1809	Fe(bcc)	>	Fe(liq)	>	Fe(fcc)	>	Fe(hcp)
>1809	Fe(liq)	>	Fe(bcc)	>	Fe(fcc)	>	Fe(hcp)

Figure 40 shows the fitted curve and the Gibbs energy differences between Fe(bcc) and Fe(fcc) from 864 to 1184 K. The twelve values were extracted from the literature in an analysis of alloy chemistry by Prof. Hillert (1986) and supplied for inclusion among the fitted data. The largest departure of the function from the data is 23 J/mol at 1013 (Hasabe and others, 1985). For the 10 remaining data, the average error is 7.1 J/mol.

Figure 41 shows the fitted function (line) and the evaluations by Bendick and Pepperhoff (1982), Chuang and others (1985), Orr and Chipman (1967), and Tsuchiya and others (1971). Compilations such as the JANAF Thermochemical Tables, (Chase and others, 1985) and Hultgren and others (1973), are essentially the same as the compilation by Orr and Chipman (1967). Above 1050 K all evaluations are equivalent. Below 1050 the fitted function is closest to the evaluations by Orr and Chipman and by Chuang and others.

From vapor pressure observations, Stepakoff and Kaufman (1968) determined that the Gibbs energy difference for the inversion Fe(fcc) to Fe(hcp) was +4,279 J/mol ("+" on Figure 42). The results of Stepakoff and Kaufman's evaluation are shown as "o" on Figure 42. The results of this review are shown as a line. The correlation is acceptable.

VOLUME OF THE SOLIDS

To obtain a reasonable description of the phase equilibria at elevated pressures, the molar volumes, expansivities, and compressibilities are needed. Table 8 gives the molar volumes and densities for the three solids at 1 bar from 200 to 3000 K and for the liquid from 1000 to 3000 K. The molar volumes are plotted on Figure 43. The fitting function is as follows:

$$V(T,P) = [V_0\ e^{\int alpha} + V(M)]\cdot[1 + b_6\ P/(b_4 + b_5\ T)]^{-(1/b_6)} \qquad 16.$$

where V_0 is the constant b_7 on Table 1 and is the constant of integration, alpha is the cubic expansion coefficient at the zero pressure, V(M) is the contribution to the volume caused by the disordering of the magnetic structure, b_6 is n and $(b_4+b_5\ T)$ is the isothermal bulk modulus as given in the Murnaghan equation. V_0 is always less than than V(298,1). The cubic volume coefficient at zero pressure was modelled using the following function:

$$alpha = b_1 + b_2\ T + b_3\ e^{(-T/b_8)} \qquad 17.$$

where b_1 through b_3 are fitted constants and b_8 is an empirical constant. For iron, b_8 was set to 650 K because it gave the best fit of the available data. (Without data available, a trial constant to use for b_8 would be 1.5 x T_D where T_D is the Debye temperature evaluated at temperatures near 0 K.) For the solids, b_2 was set to zero; for liquid, b_3 was set to zero. For the solids, the function approaches a constant as does the volume expansion coefficient at high temperatures.

For the magnetic anomaly, it was postulated that the anomaly in volume was similar to the anomaly in enthalpy. Plots of these properties appeared to be of the same form. Therefore, the following relation was assumed.

$$V(M) = a_{12}\, H(M) \qquad 18.$$

This assumption is in good agreement with the data and with the critical temperature as a function of pressure. The latter will be discussed below.

What follows is a study-by-study review of the volume-related data available at the time of this compilation.

Basinski and others (1955). The molar volume was measured by X-ray techniques between 293 and 1775 K at ambient pressure. The experimental data and the fitted functions for Fe(bcc) and Fe(fcc) are shown on Figure 44. The data were part of the fitted file and the largest error is 0.007 cm^3/mol at 1662 K. The average error is 0.002 cm^3/mol.

Benkisser (1980). The volume of Fe(hcp) at 298 K and 1 bar was estimated to be 6.796 cm^3/mol from an analysis of iron-manganese alloys. The fitted value is 6.870 cm^3/mol, a difference of 0.11 cm^3/mol.

The volume of Fe(fcc) at 298 K and 1 bar was found to be 6.860

cm^3/mol. The fitted value was found to be 6.853 cm^3/mol with an error of 0.007 cm^3/mol.

Besson and others (1988). From X-ray measurements in high-pressure diamond cells, the molar volume of Fe(fcc) was found to be 6.01 cm^3/mol at 2300 K and 420 kbar. The fitted volume is 6.36 cm^3/mol, an error of 0.35 cm^3/mol.

Blackburn and others (1965). The molar volumes of the iron polymorphs were estimated from studies of the iron-ruthenium alloys to be as follows:

POLYMORPH	ESTIMATED VOLUME	CALCULATED VOLUME	REMARKS
Fe(bcc)	7.11	7.0918	
Fe(fcc)	7.27	6.853	The two values correspond to high-moment high-volume and low-moment low-volumes respectively.
	6.745		
Fe(hcp)	6.781	6.870	

The data were given zero weight in the fitting.

Brown and McQueen (1986). From shock experiments, the volume of Fe(hcp) was found to be as follows:

TEMPERATURE† (K)	PRESSURE (kbar)	VOLUME MEASURED (cm^3/mol)	VOLUME FITTED (cm^3/mol)
786	400	5.885	5.887
1163	600	5.590	5.672
1626	800	5.370	5.515
2154	1000	5.200	5.387
2729	1200	5.059	5.266
3340	1400	4.942	5.133
3973	1600	4.839	4.966
4625	1800	4.753	4.733

† The temperatures were adjusted to be in agreement with the experimental data of Williams and others (1987).

The last column gives the calculated volumes. The largest error is 0.21

cm^3/mol and the agreement is acceptable. It must be noted that the first-order Murnaghan equation was never intended for use up to these confining pressures.

Clendenen and Drickamer (1964). Figure 45 shows the results of early experiments on the molar volume of Fe(bcc) and Fe(hcp) as a function of pressure at 298 K. The early results were given zero weight in the optimization.

Donohue (1974). A critical review of the lattice constants by Donohue at 293.15 K yielded a value of 7.0912-0.0014 cm^3/mol. This review found 7.0905-0.001 cm^3/mol.

Esser and Mueller (1933). The reported data are systematically low by 0.04 cm^3/mol and were given zero weight. Figure 46 is a plot of the reduced volumes, V(T)/V(293). The data trend toward higher volumes with increasing temperature.

Fasiska and Zwell (1967). X-ray techniques were used to measure molar volumes of Fe(bcc) at 296, 687, and 951 K. The data, plotted on Figure 47 ("+") were fit with errors of 0.000, 0.003, and 0.000 cm^3/mol, respectively.

Giles and others (1971). The molar volume of Fe(bcc) and Fe(hcp) were measured to 163 Kbar at 300 K (Figure 48). The data were given zero weight in the optimization. The reduced volumes for Fe(bcc) appear to be acceptable but the data for Fe(hcp) indicate a systematically smaller molar volume of about 0.04 cm^3/mol.

Goldschmidt (1962). X-ray techniques were used to measure molar volumes of Fe(bcc) and Fe(fcc) from 293 to 1528 K. Refer to Figure 49 for a plot and fit of the data. The data were used in making this optimization and the largest error is 0.010 cm^3/mol at 1528 K. The average error in volume for Fe(bcc) is 0.002 cm^3/mol and for Fe(fcc) is 0.007 cm^3/mol.

Gorton and others (1965). X-ray techniques were used to measure molar volumes between 295 and 1343 K. The data are plotted on Figure 50. Because the data were anomalously high, the data were given zero weight in this review.

Huang (1987); Huang and others (1987). In his dissertation Huang measured the molar volume of Fe(bcc) and Fe(hcp) to 723 K and 240 kbar using high-pressure diamond cells and synchrotron radiation. Refer to Figure 51 for a plot of the experimental data and the fitted curves. For Fe(bcc) only the 723 K isotherm is anomalous when the precision of the data is considered. For Fe(hcp) the data below 150 Kbar on the 423- and 723-K isotherms are anomalous. The other data were used in the fit but the precision was set at 0.02 cm^3/mol.

Jack (1951). From an analysis of the data in the Fe-N system, the volume of Fe(fcc) was found to be 6.856 cm^3/mol at 298 K and 1 bar. The fitted value is 6.853 cm^3/mol.

Jephcoat and others (1986). Molar volumes were measured by X-ray techniques in diamond cells to near 800 kbar at 298 K. The reduced volumes are plotted on Figure 52 along with the fitted curves The values for Fe(hcp) below 200 kbar were given zero weight because the data have an anomalous trend. The other data were fit within the precision reported by Jephcoat and others.

Kochanovska (1949). X-ray techniques were used to measure the volume of Fe(bcc) from 295 to 639 K. Because the data appear to have a systematic error of about -0.04 cm^3/mol, the values were converted to reduced volumes [=V(T)/Vr(295)]. Because of the systematic error shown on Figure 53, the data were given zero weight.

Kohlhaas and others (1967). Molar volumes between 93 and 1781 K were measured using X-ray techniques and reported. Refer to Figure 54. The data for Fe(bcc) is satisfactory except near T_c at 1043 K. From about 980 to greater than 1184 K, the observed volumes are anomalously low by 0.02 cm^3/mol and indicate a larger volume change caused by the magnetic disordering. For Fe(fcc), the volumes have an anomalous trend. The data were given zero weight in this evaluation. The volume is high at 1223 K by 0.01 cm^3/mol and is low at 1634 K by 0.02 cm^3/mol.

Mao and Bell (1979). Molar volumes between 437 and 941 kbar were measured at 298 K using X-ray techniques and high-pressure diamond cells. The data are plotted as reduced volumes on Figure 55. The fitted function is consistent with the data within the precision of the measurements.

Mao and others (1967). Molar volumes at 296 K were measured to 309 kbar by X-ray techniques and high-pressure daimond cells. The data are plotted as reduced volumes on Figure 56. The data were used in this evaluation and fit within the precision of the observations.

Newkirk (1957). From an analysis of the data in the Fe-Cu system, the volume of Fe(fcc) was found to be 6.954 cm^3/mol at 298 K and 1 bar. The fitted value is 6.853 cm^3/mol.

Owen and Williams (1954); Owen and Yates (1937). X-ray techniques were used to measure the volumes of iron from 79 to 913 K. There appeared to be a systematic error of -0.04 cm^3/mol in these studies. Therefore the data were converted to reduced volumes [=V(T)/Vr(295)] prior to fitting.

Figure 57 shows the reduced volumes as a function of temperature. The observation at 913 K was given zero weight because of the indicated anomalous increase in the expansivity. The largest error is 0.004 cm^3/mol at 79 K. The average error is 0.001 cm^3/mol.

Paranjpe and others (1950). From an analysis of the data in the Fe-N system, the volume of Fe(fcc) was found to be 6.862 cm^3/mol at 298 K and 1 bar. The fitted value is 6.853 cm^3/mol.

Ridley and others (1969); Ridley and Stuart (1970). Figure 58 shows the data for Fe(fcc) estimated from an analysis of the Fe-C system. The maximum error is 0.02 cm^3/mol at 298 K and the average error is 0.01 cm^3/mol. Except for the data at 1273 and 1473 K, these data represent a metastable phase.

Robie and others (1979). The compilation of thermodynamic data list the molar volume of Fe(bcc) as 7.092 cm^3/mol. The fitted value from this study is 7.0918 cm^3/mol.

Ruhl and Cohen (1969). From experimental measurements in the Fe-C system, the molar volume of Fe(hcp) at 298 K and 1 bar was found to be 6.805 cm^3/mol. Ruhl and Cohen also cited unpublished research by G.L. Stepakoff where he obtained the molar volume of 6.829 cm^3/mol from experimental work in the Fe-Rh system. The fitted volume is 6.687 cm^3/mol.

Straumanis and Kim (1969). X-ray techniques were used to measure volumes of alpha-iron between 283 and 337 K (tabular data were supplied in the manuscript) and between 523 and 1423 K (equations only supplied). Refer to Figure 59. The experimental data were used in the optimization whereas the values calculated from their equations were not because data smoothed by one equation and then refit by a different equation may be unreliable. The maximum error of the fitted data is 0.007 cm^3/mol and the average is 0.004 cm^3/mol.

Stuart (1988); Ridley and Stuart (1968). X-ray techniques were used to measure volumes of Fe(bcc) from 292 to 1161 K. The data and the fitted curve is shown on Figure 60. The data were used in making this optimization. The maximum error is 0.005 cm^3/mol at 813 K and the average error is 0.002 cm^3/mol.

Takahashi and others (1968). Experimental molar volumes were measured to 300 kbar at 296 K using X-ray techniques and high-pressure diamond cells. The data, plotted as reduced volumes, are plotted on Figure 61. The fitted equations are in good agreement with the experimental data.

von Bachelder and Raeuchle (1954). The molar volumes were measured by X-ray techniques from 298 to 673 K. Unfortunately, only the experimental value at 298 K was given explicitly. The values given on Figure 47 ("o") were scaled from Figure 1 of the published manuscript. Because only scaled data were available, a precision larger in magnitude and, therefore, a lower weight was assigned to these data. The largest error between the "observed" and the calculated values is 0.004 cm^3/mol at 523 K. The average error is 0.001 cm^3/mol.

Watanabe and others (1981). A sessile drop method was used to measure the density of Fe(bcc) and Fe(fcc) from 673 to 1812 K. The data, supplied by the authors as equations, are plotted on Figure 62. The data, given a relatively low weight, were fit with a maximum error of 0.009 cm^3/mol at both 673 and 1184 K. The average error is 0.004 cm^3/mol which is well within the experimental precision of the data.

VOLUME OF THE LIQUID PHASE

Table 9 and Figure 63 summarize the data for Fe(liq) used in this study. The data flagged with an asterisk (*) were included in the optimization. The other data were given zero weight. The maximum and average errors, respectively, are given in the last two columns of Table 9. The fitted curve is an acceptable synthesis of the experimental data.

CUBIC EXPANSION COEFFICIENT

Figure 64 shows the fitted cubic expansion coefficients at 1 bar total pressure. Table 10 gives the data for the solids from 200 to 3000 K and for the liquid from 1000 to 3000 K. These results are based on a fit of the volumes given above and data given in several of the references cited below in a study-by-study summary (Figure 65).

Cleaves and Hiegel (1942). Cubic expansion coefficients (converted from linear expansion coefficients) were reported from 298 to 523 K. The error in fitting the data was generally less than 1 percent. The data were given zero weight because the data indicated a linear relation with temperature. Such a relation is not to be expected in this temperature region. Also, the data were the results of mechanical measurements of length. X-ray determinations are preferred for thermodynamic correlations.

Fraser and Hollett (1961). Data were reported from 20 to 300 K. However, only the data at 150 K and above were included in this optimization. The data were fit with an error of 10 percent at 150 K and under 2 percent at 300 K.

Richter (1970). Richter reported data from 81 to 1773 K. In the optimization, the data were given zero weight because the data are based on dilatometric measurements. X-ray techniques are to be preferred. The data above T_C appear to be too low to allow fitting of the internally consistent molar volumes reported by Basinski and others (1955) and Watanabe (1981) for Fe(bcc). The coefficients for Fe(fcc) are also low when compared to the experimental data of Basinski and others (1955), Goldschmidt (1962), Ridley and Stuart (1970), Straumanis and Kim (1969), and Watanabe (1981).

White (1965). Coefficients were reported from 3 to 283 K. However, because the fitting function is not reliable at low temperatures, only the data at 200 and 283 K were weighted and fit with a precision of about 4 percent.

APPARENT CUBIC EXPANSION COEFFICIENT

Figures 66 and 67 show the apparent cubic expansion coefficients where:

$$\text{"alpha"} = \frac{V(T) - V(Tr)}{V(Tr)} \cdot \frac{1}{(T-Tr)} \qquad 19.$$

None of the data plotted on the figure were given weight in this evaluation because dilatometric measurements are less reliable than X-ray techniques when thermodynamic properties are needed.

Esser and Eusterbrock (1941). From dilatometric measurements, the authors reported apparent coefficients from 323 to 1138 K for Fe(bcc) and at 1223 and 1273 K for Fe(fcc). The reference temperatures for Fe(bcc) and Fe(fcc) were 18 and 900 K, respectively. The data were not used in the optimization but were fit within 3 percent of the observed.

Lehr (1956). Apparent coefficients were reported from 373 to 1123 K with the reference temperature at 293 K. The data are from dilatometry and are not consistent with the X-ray observations above. The data were given zero weight.

Nix and MacNair (1941). Dilatometry was used to report linear expansion coefficients from 92 to 957 K. The reference temperature was 273.15 K. The data are anomalous and were given zero weight because there is an apparent arrest in the thermal expansivity at 350 to just above 400 K. None should exist. Figure 67 is a plot of the observed and calculated data converted to cubic expansion coefficients. The large scatter near 273 K is due to the inaccuracy of the method for temperatures close to the reference temperature.

Richter (1970). The apparent coefficients were reported from 81 to 1173 K. The measurements were made by dilatometry and the reference temperature was 293 K (Figure 66). The data, though given zero weight, were fit within 3 percent of the reported data.

ISOTHERMAL COMPRESSIBILITY AND ISOTHERMAL BULK MODULUS

Figures 68 and 69 are plots of the isothermal compressibility and the isothermal bulk modulus at 1 bar for the three solids and for the liquid. Data on Tables 11 and 12 were calculated from the modelling equations which are, respectively:

$$\mathrm{kappa}_T = K_T^{-1} \qquad 20.$$

$$K_T = b_4 + b_5\, T + b_6\, P \qquad 21.$$

In equation 21, the effect of pressure on V(M) was not factored in. The equations are complex and the error in neglecting "$V^{-1}\cdot dV(M)/dP$" is small.

The parameters supplied here were obtained by fitting of all data in the data file. Boehler (1988) reported in an abstract that he derived values for the isothermal bulk modulus for Fe(fcc) at 0 bars that varied from 1.75 Mbar at room temperature to 0.81 Mbar at 2000 K. From this study, the calculated values are 1.55 and 1.04 Mbars, respectively. Boehler's reported data may be in error. There is evidence that the reported pressures in related studies by Boehler (1986) and Boehler and others (1986,1987) are high and not consistent with the thermal functions and the volumetric properties. For example, refer to Figures 76 and 79.

ISENTROPIC COMPRESSIBILITY AND ISENTROPIC BULK MODULUS

Figures 70 and 71 are plots of the isentropic compressibility and the isentropic bulk modulus at 1 bar for the solids and for the liquid. Data on Tables 13 and 14 were calculated from the modelling equations which are, respectively:

$$\text{kappa}_S = \text{kappa}_T - \frac{\alpha^2\, V\, T}{10\, C_p} \qquad 22.$$

$$K_S = \mathrm{kappa}_S^{-1} \qquad 23.$$

where alpha and V are given by equations 17 and 16 above and C_p is given by equation 2 above.

The isentropic bulk modulus may be calculated from the experimentally measured elastic constants.

$$K_S = (c_{11} + 2\ c_{12})/3 \qquad 24.$$

Lord and Beshers (1965) derived the elastic constants from accoustic measurements between 70 and 417 K. From their data, the isentropic bulk modulus at 77 and 298 K are 1.68 and 1.64 Mbar, respectively. At 298 K the calculated isentropic bulk modulus is 1.62 Mbar. It is not appropriate to calculate the value at 77 K because the temperature is below the fit-range of this study.

Dobretsov and Peresada (1971) reported a value of 1.663 (±0.018) Mbar as the isentropic bulk modulus and 4.94 (±0.25) as the first pressure derivative. In this study, the calculated isentropic bulk modulus and the first pressure deribative are 1.623 Mbar and 7.02, respectively. The difference is assigned to the use of the Murnaghan equation of state in this study as a fitting equation and not as a virial equation of state. In this study, the intention was to fit as large a pressure range as possible with a minimum of constants.

Filippov and others (1966) derived 0.74 Mbar^{-1} as the isentropic compressibility at 1825 K from accoustic measurements. The calculated value is 0.87 Mbar^{-1} and is in acceptable agreement.

Figure 72 shows the fitted curve and the additional isentropic bulk moduli for Fe(bcc) as derived from ultrasonic experiments. The data show that the modelling of the bulk modulus is somewhat flawed. There are two approaches that are required to improve the fit. First, a more complex equation than the first-order Murnaghan equation would be required. With a function of higher order, the additional constants would allow better fit of the data at "zero" pressure. Secondly, the temperature dependence of these constants should be modelled better than the linear dependence used here for K_T.

THE CRITICAL TEMPERATURE

The critical temperature for the Neel transition in Fe(fcc) was taken from the study of Fernandez Guillermet and Gustafson (1985) without modification.

$$T_N[\text{Fe(fcc)}] = 67\ \text{K}. \qquad 25.$$

Magnetic ordering in Fe(hcp) has not been found (Williamson and others, 1972; Cort and others, 1982).

For Fe(bcc), there are three studies of the Curie temperature that report T_C as a function of pressure. They are plotted on Figure 73 along with the fitted curve. Only the data of Mirwald and Kennedy (1979) were used in this study because only they were consistent in slope with the fitted magnetic contributions to entropy and volume at "zero" pressure:

$$\frac{d\,T_c}{dP} = 0.1\,\frac{V(M)}{S(M)} = 0.1\,\frac{T_c\,V(M)}{H(M)} \qquad 26.$$

Substituting for V(M), as given in equation 18 above,

$$\frac{d\,T_c}{dP} = 0.1\,a_{12}\,T_c \qquad 27.$$

The fitted equation for the critical temperature is

$$T_c = a_{11}[1 + 0.1\,a_{12}(P - 1)] \qquad 28.$$

where a_{11} is the critical temperature at 1 bar and a_{12} is the slope. In the fitting, a_{12} was forced to be consistent with equation 18 above also.

PHASE EQUILIBRIA AT ELEVATED PRESSURES

The equations describing the thermal functions and the molar volumes were combined to calculate the phase equilibria as shown on Figure 74. The equilibria were calculated by searching for the pressures and temperatures where the following identity was valid.

$$\Delta_i G(T,P) = 0 = \Delta_i G(T,1) + 0.1 \int_1^P \Delta V\, dP \qquad 29.$$

The conversion factor of 0.1 is used because volumes are expressed in cm^3/mol and not J/(bar mol).

The invariant points are located at 754 K and 102 kbar (point A, liquid absent equilibria) and at 1979 K and 50 kbar (point B, Fe(hcp) absent equilibria).

Figure 75 shows the fit and the data that were used in the optimization. Figures 76 and 77 show those data that were given zero weight in the optimization. The data for Fe(bcc) = Fe(fcc) equilibria as measured by Kennedy and Newton (1963), Strong and others (1973), and Mirwald and Kenedy (1979) are in excellent agreement with the thermal functions at 1 bar. By contrast, the data plotted on Figures 76 and 77 could not be forced to be compatible with the known volumes and thermal functions at 1 bar and the available molar volumes at elevated pressures.

The same is true for the equilibrium reactions Fe(bcc) = Fe(hcp) and Fe(fcc) = Fe(hcp). Attempts to give greater weight to the work of Boehler (1986) and Boehler and others (1986,1987) or to Manghnani and others (1987) and Manghnani (1988) caused unacceptable compensating distortions in the molar volumes and in the thermal functions.

Figures 78a and 78b are plots of the data used to define the equilibria around the invariant point at "B". Figure 78b shows the same equilibria as on Figure 78a but the scale was adjusted so that the reversals for the melting of Fe(fcc) up to 1 Mbar could be plotted clearly. The equilibrium curve for that reaction was only plotted to 200 kbar because the mathematical model fails beyond that point. The calculated volume difference between Fe(fcc) and Fe(liq) becomes negative. Plotted on Figure 79 are the observed equilibria that were given zero weight in the optimization. It appears that the pressure calibration was too high or the temperature measurement was too low for the equilibria as measured by Boehler (1966).

SUMMARY

The review produced a superior set of internally consistent equations describing the properties of Fe(bcc), Fe(fcc), Fe(hcp), and Fe(liq) over the temperature ranges where data are available. The improvements include the following:

1. The heat capacity of Fe(bcc) is consistent with the estimated contribution to S(T) from the disordering of the magnetic structure.
2. The enthalpy differences among the polymorphs agree with the phase equilibria at 1 bar.
3. The calculated volumes of all phases agree with the experimental data. This is a step forward for Fe(bcc) because the contribution at the Curie temperature is included in the equations.
4. The location of the critical temperature as a function of pressure has been tied in with the one-bar data for H(M) and V(M).

5. The phase equilibria among the solids are fit to 500 kbar. The phase equilibria between the solids and the liquid were fit to 200 kbar.

Two minor difficulties must be noted. They are being left for future studies.

1. The calculated isentropic bulk modulus does not agree perfectly with the data. Refer to Figure 72.

and 2. The functions fail to calculate the equilibrium Fe(fcc) = Fe(liq) at high pressures (above 200 kbar).

SUGGESTIONS FOR FUTURE IMPROVEMENTS

One would be remis if suggestions for improvements were not advanced after a detailed evaluation. Concerning additional experimental data, the following studies would greatly improve the evaluation:

1. Molar volumes (or densities) for both Fe(fcc) and Fe(liq) at elevated temperatures to pressures as high as possible.

and 2. Elastic constants and isentropic bulk moduli for Fe(fcc) and Fe(liq) at zero or ambient presure.

Both of these sets of data are needed to better describe the properties of the phases as a function of pressure and temperature. The thermal data and molar volumes at one bar are adequate.

Although not fully a part of this study, a "small" improvement to S°(298.15,1) would result from a Cp° study from 5 to 350 K. It is unfortunate that there is no reliable study that covers this complete temperature range.

Concerning the review process, the next evaluation (to be made after the above data are available) should use an equation of higher order. The first-order Murnaghan equation was used here. With additional terms, the problem of fitting the isentropic bulk modulus will not exist. Presently there are enough data for Fe(bcc) and Fe(hcp) to warrant a higher-order function for stress but there are few data other than phase equilibria to guide the fitting of the isothermal bulk modulus and its derivatives with temperature and pressure.

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We would also like to thank the many authors and editors who arranged for the publication of the cited experimental observations. The experimental observations are the only base that is adequate for a critical review. An experimental observation is a fact. If recorded correctly, it will not change with time or place. Interpretations and evaluations are subject to 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 might be considered as so much arm-waving. The conclusions become significant only if they stand the test of time through repeated analysis of the contained data and of additional data.

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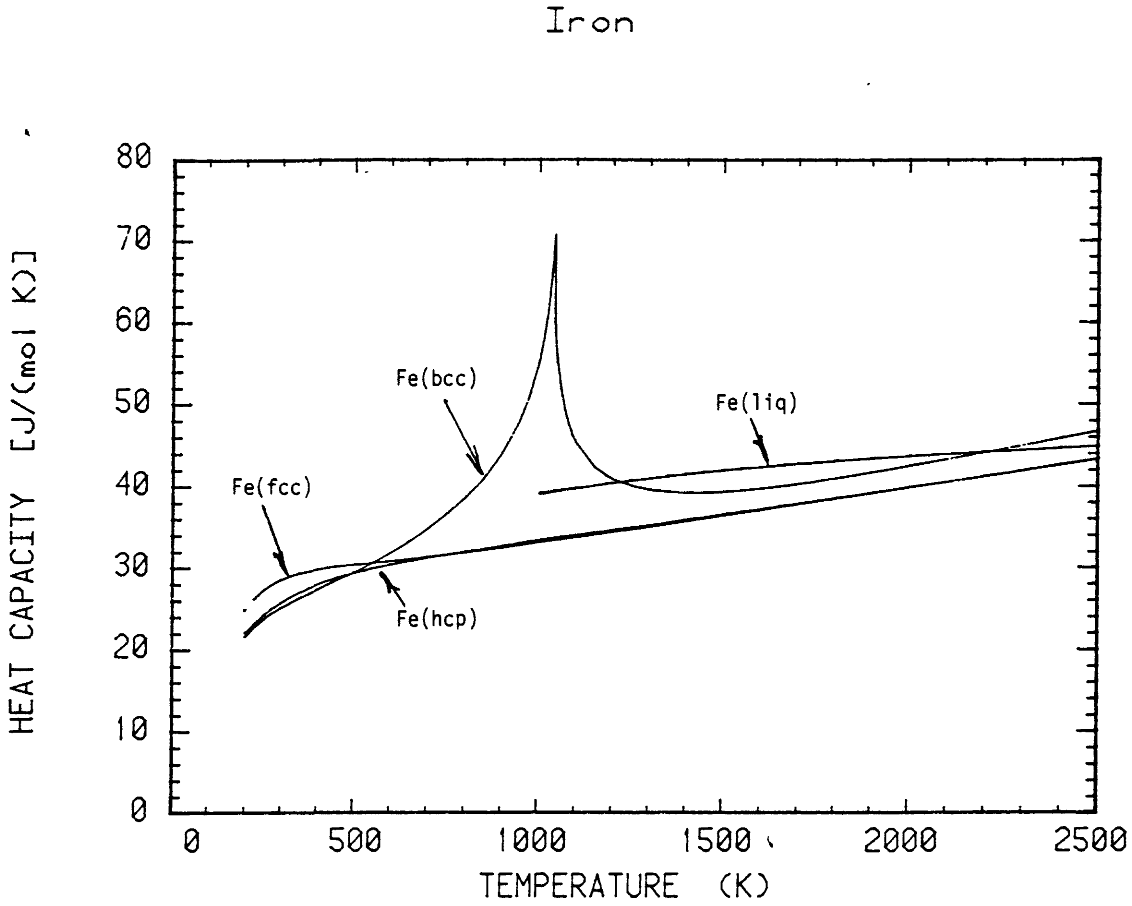


Figure 1. Heat capacity for the three solids and for the liquid as calculated from equation 2 and the constants from Table 1.

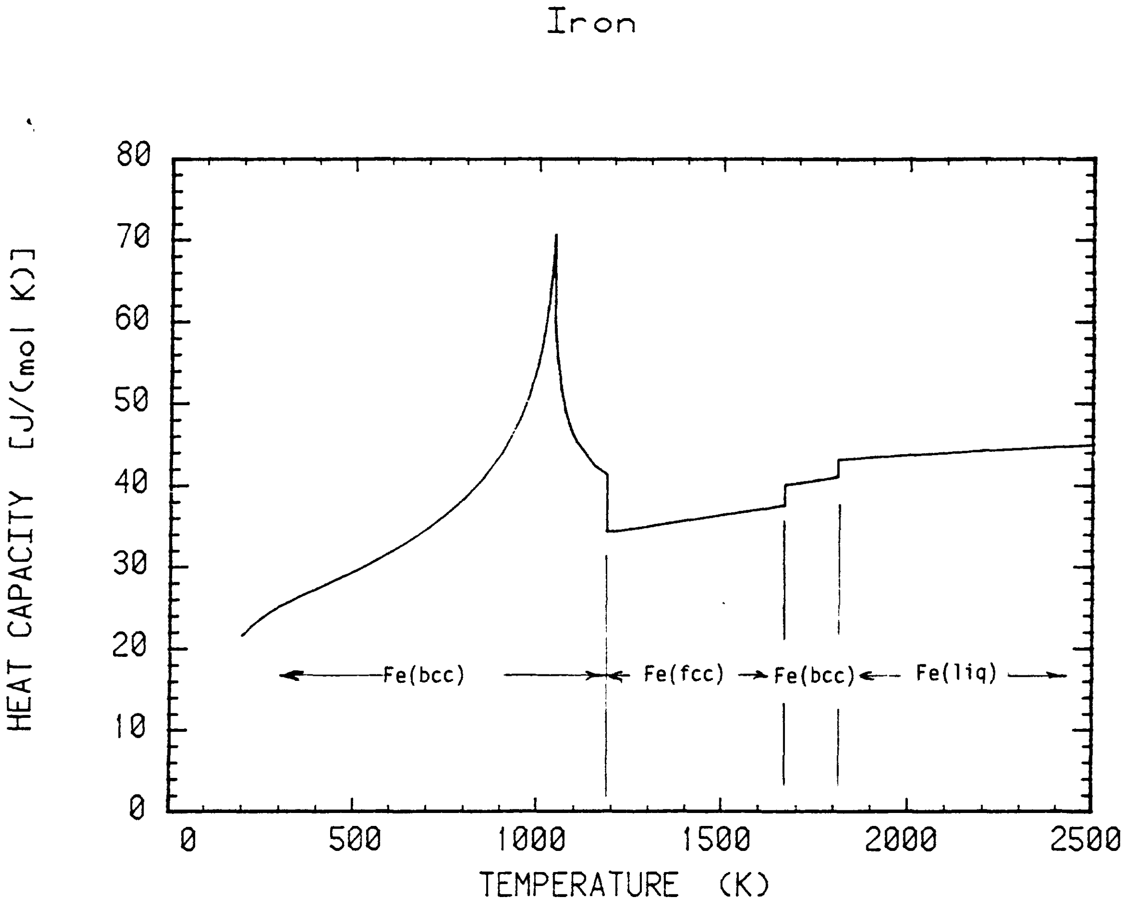


Figure 2. Heat capacity for the stable phases at 1 bar total pressure.

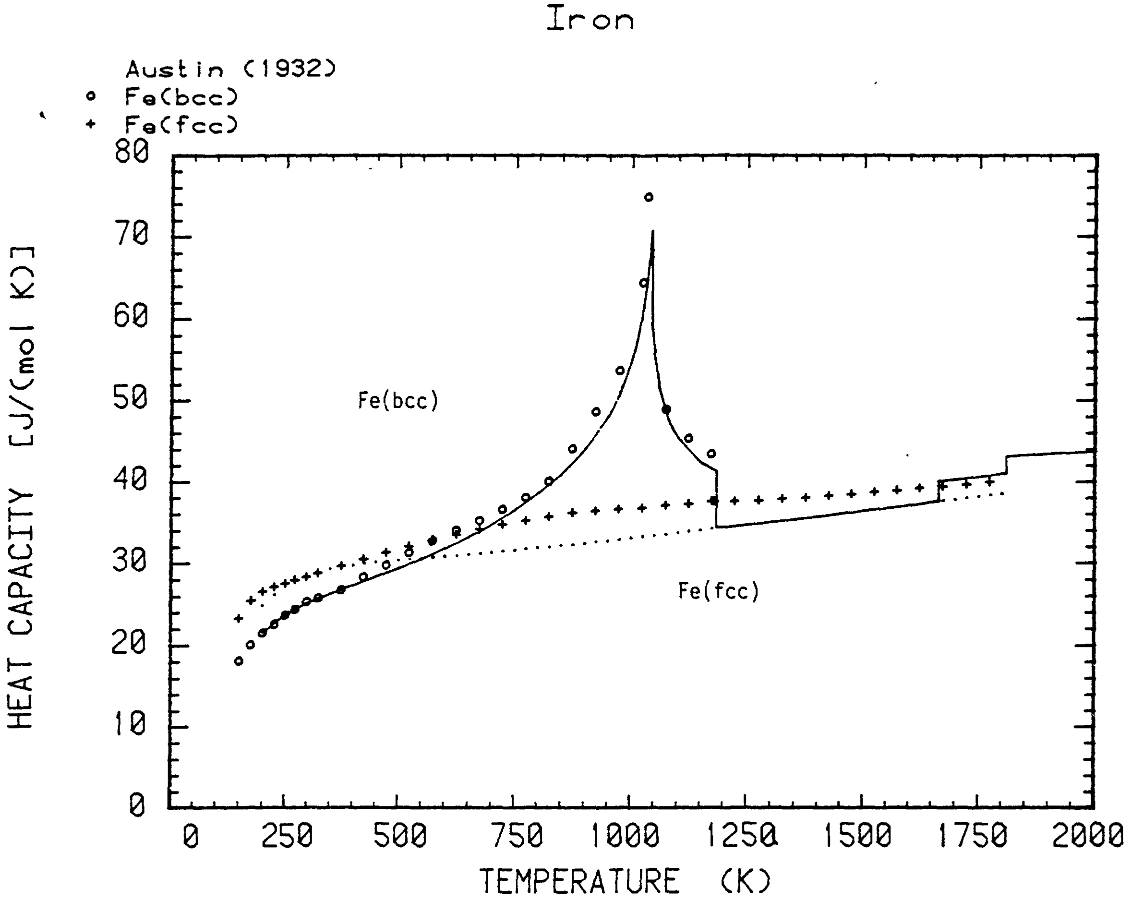


Figure 3. Comparison of the calculated heat capacities with the estimates for Fe(bcc) and Fe(fcc) as reported by Austin (1932). The solid line shows the calculated heat capacity for the stable phases. The dotted lines are the metastable extensions of the heat capacity for Fe(fcc).

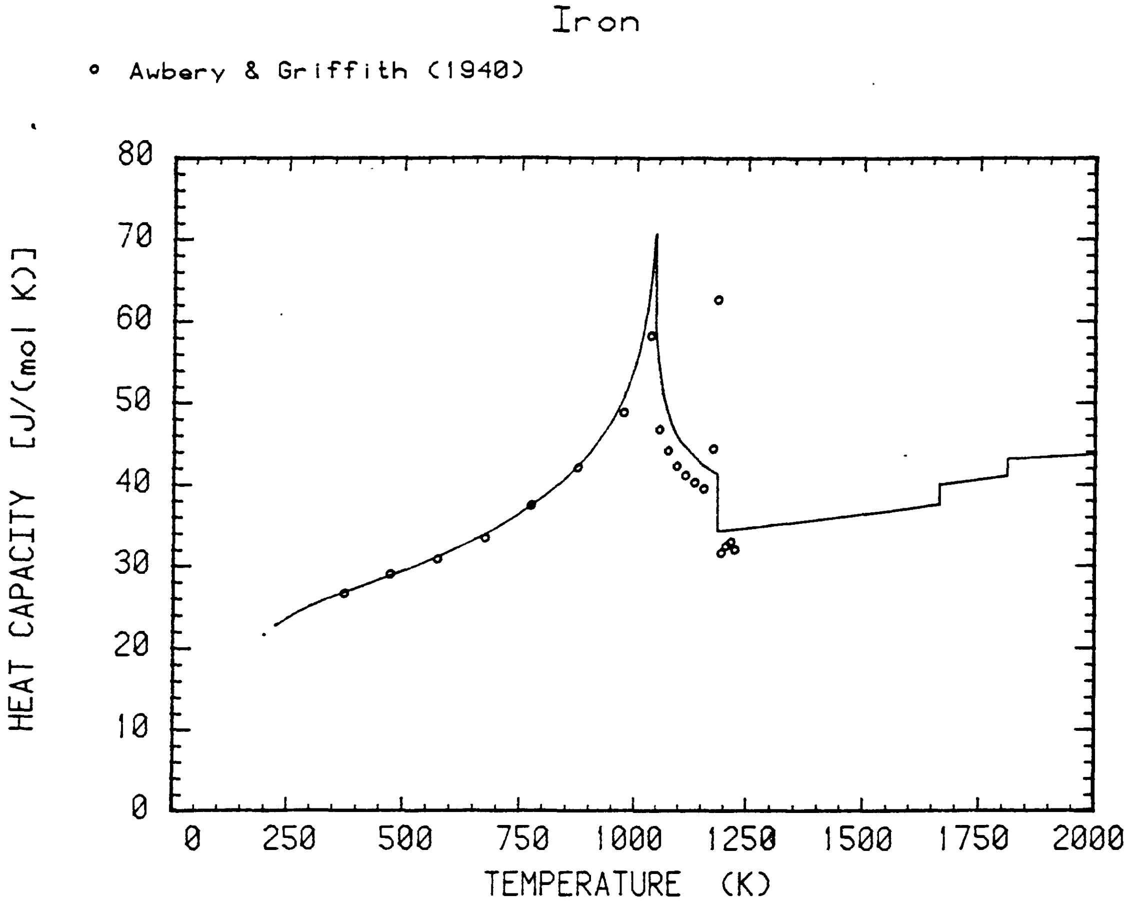


Figure 4. Comparison of the calculated heat capacities with the experimental data for Fe(bcc) and Fe(fcc) as reported by Awbery and Griffith (1940). The solid line shows the calculated heat capacity for the stable phases.

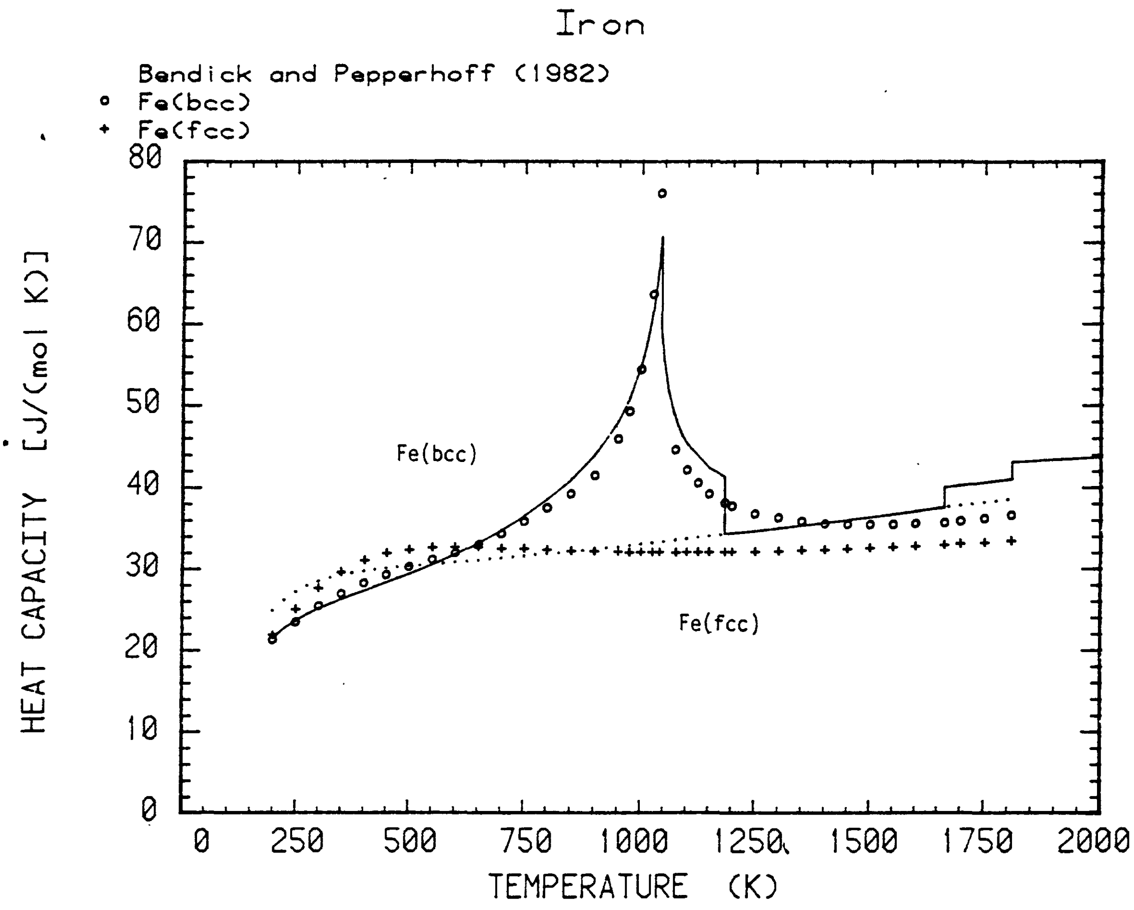


Figure 5. Comparison of the calculated heat capacities with the experimental data and estimates for Fe(bcc) and Fe(fcc) as reported by Bendick and Pepperhoff (1982). The solid line shows the calculated heat capacity for the stable phases. The dotted lines are the metastable extensions of the heat capacity for Fe(fcc).

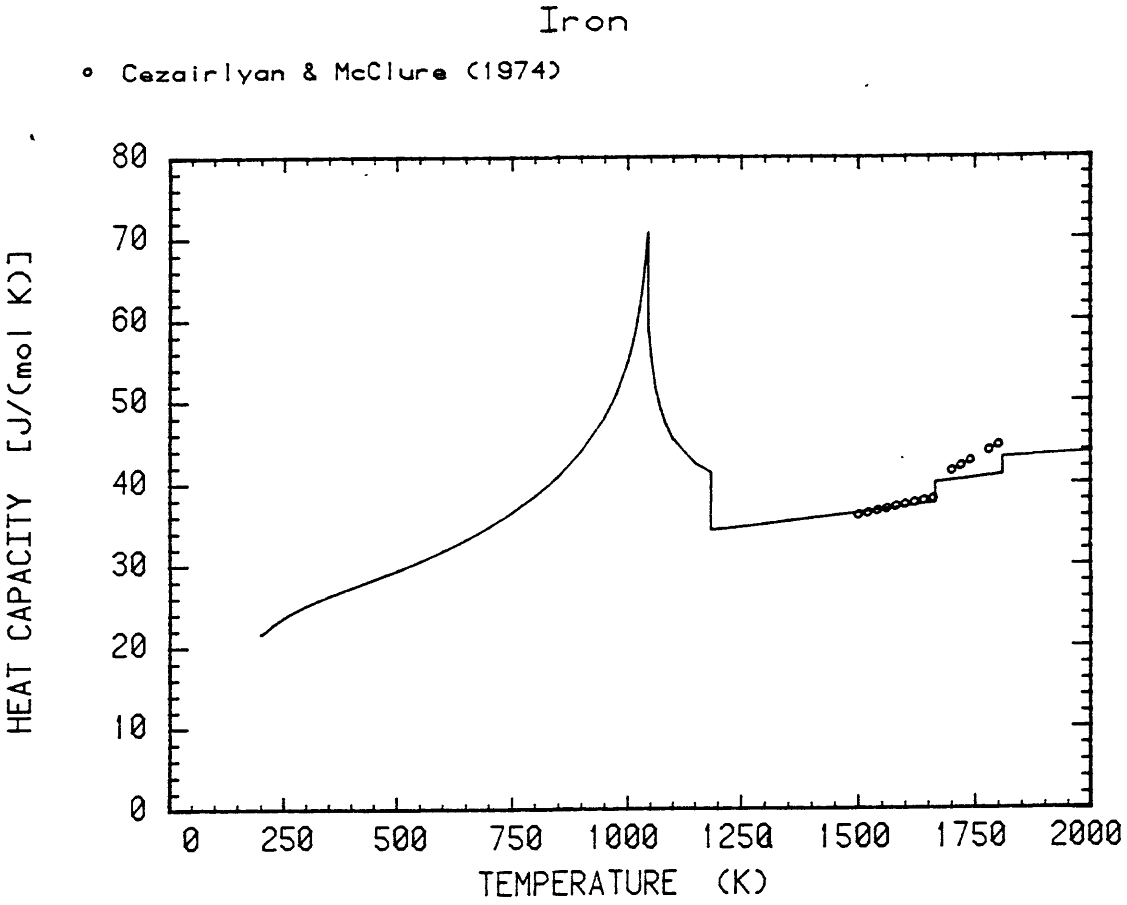


Figure 6. Comparison of the calculated heat capacities with the experimental data for Fe(fcc) and Fe(bcc) as reported by Cezairlyan and McClure (1974). The solid line shows the calculated heat capacity for the stable phases.

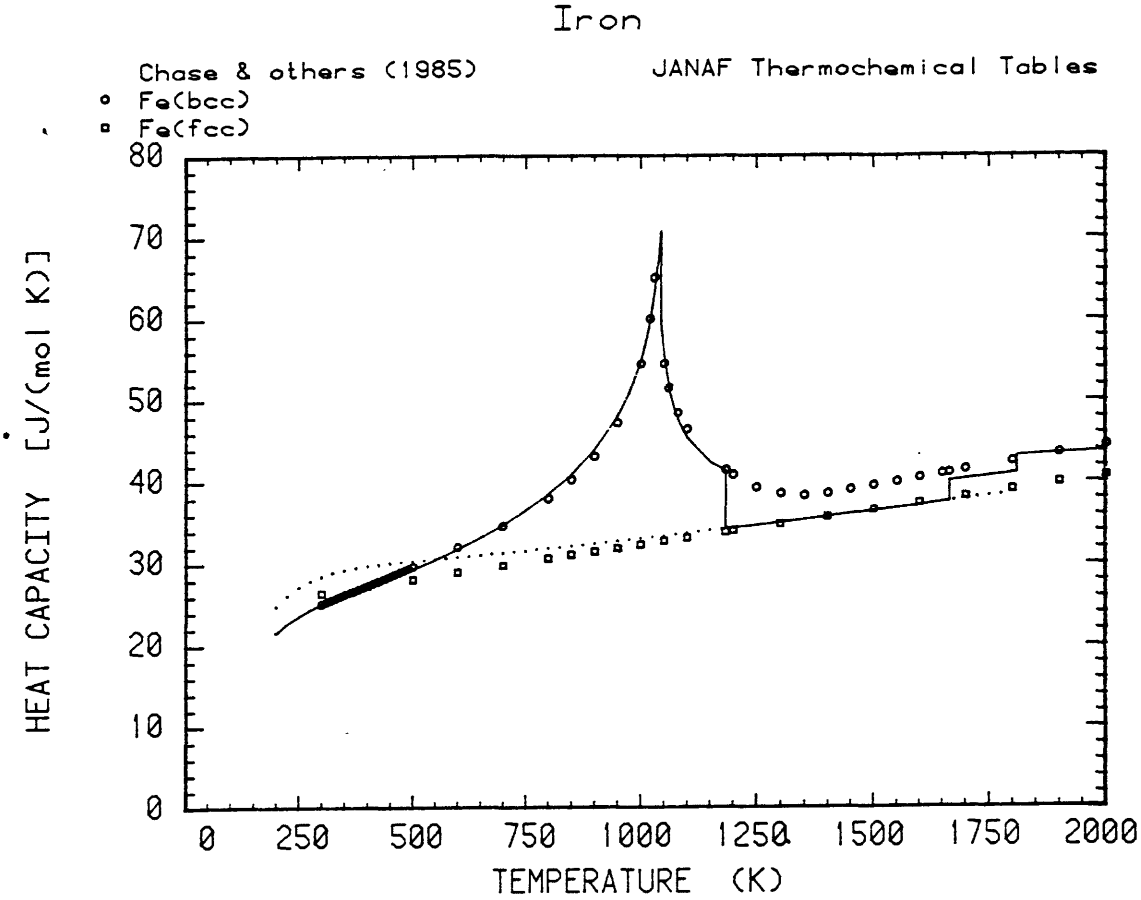


Figure 7. Comparison of the calculated heat capacities with the estimates for Fe(bcc) and Fe(liq) as reported by Chase and others (1985). The solid line shows the calculated heat capacity for the stable phases. The dotted lines are the metastable extensions of the heat capacity for Fe(fcc).

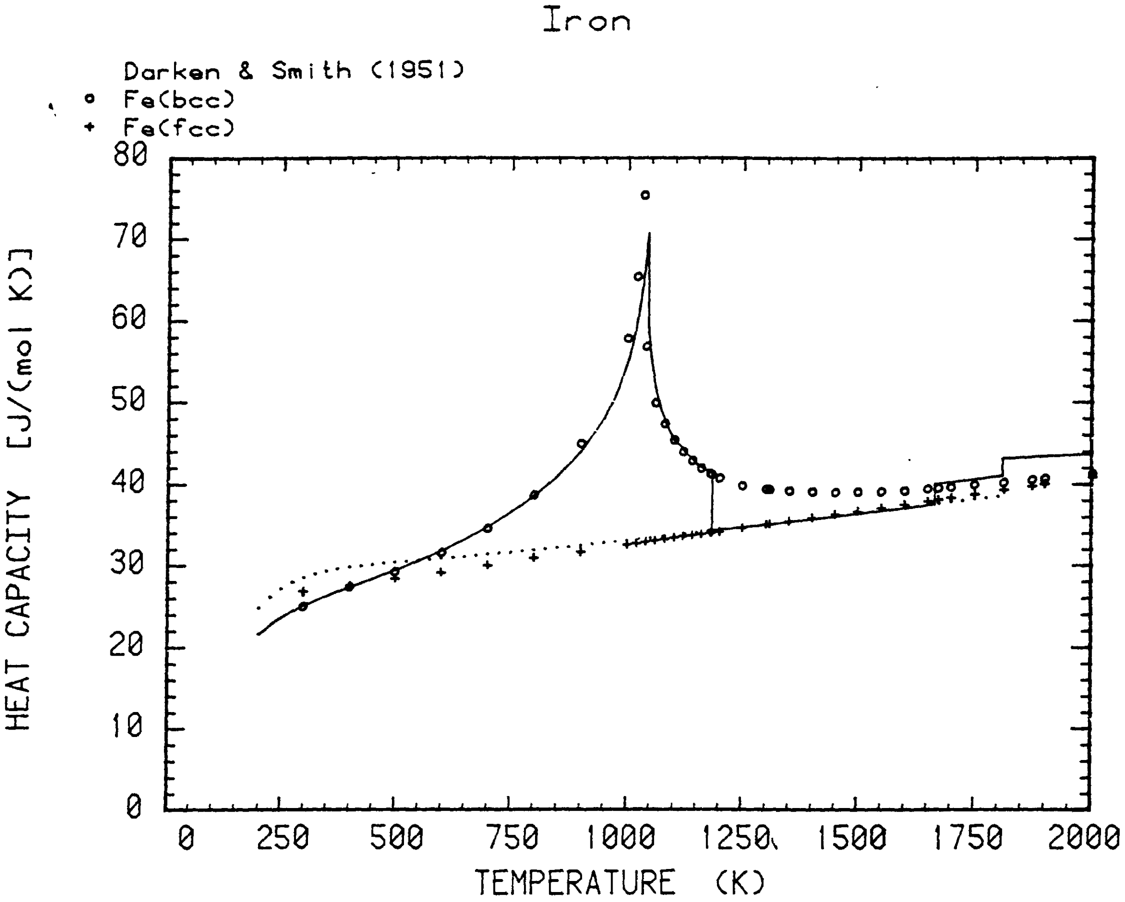


Figure 8. Comparison of the calculated heat capacities with the estimates for Fe(bcc) and Fe(fcc) as reported by Darken and Smith (1951). The solid line shows the calculated heat capacity for the stable phases. The dotted lines are the metastable extensions of the heat capacity for Fe(fcc).

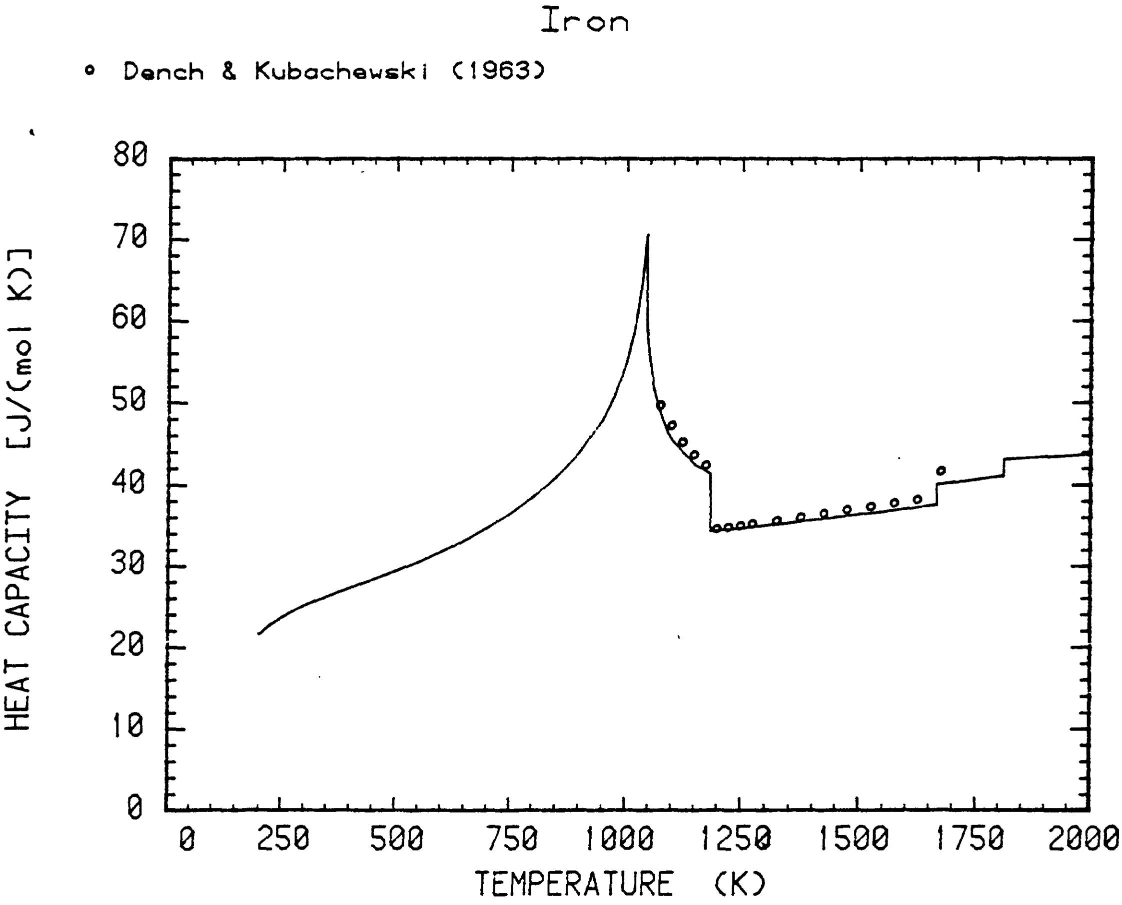


Figure 9. Comparison of the calculated heat capacities with the experimental data for Fe(bcc) and Fe(fcc) as reported by Dench and Kubachewski (1963). The solid line shows the calculated heat capacity for the stable phases.

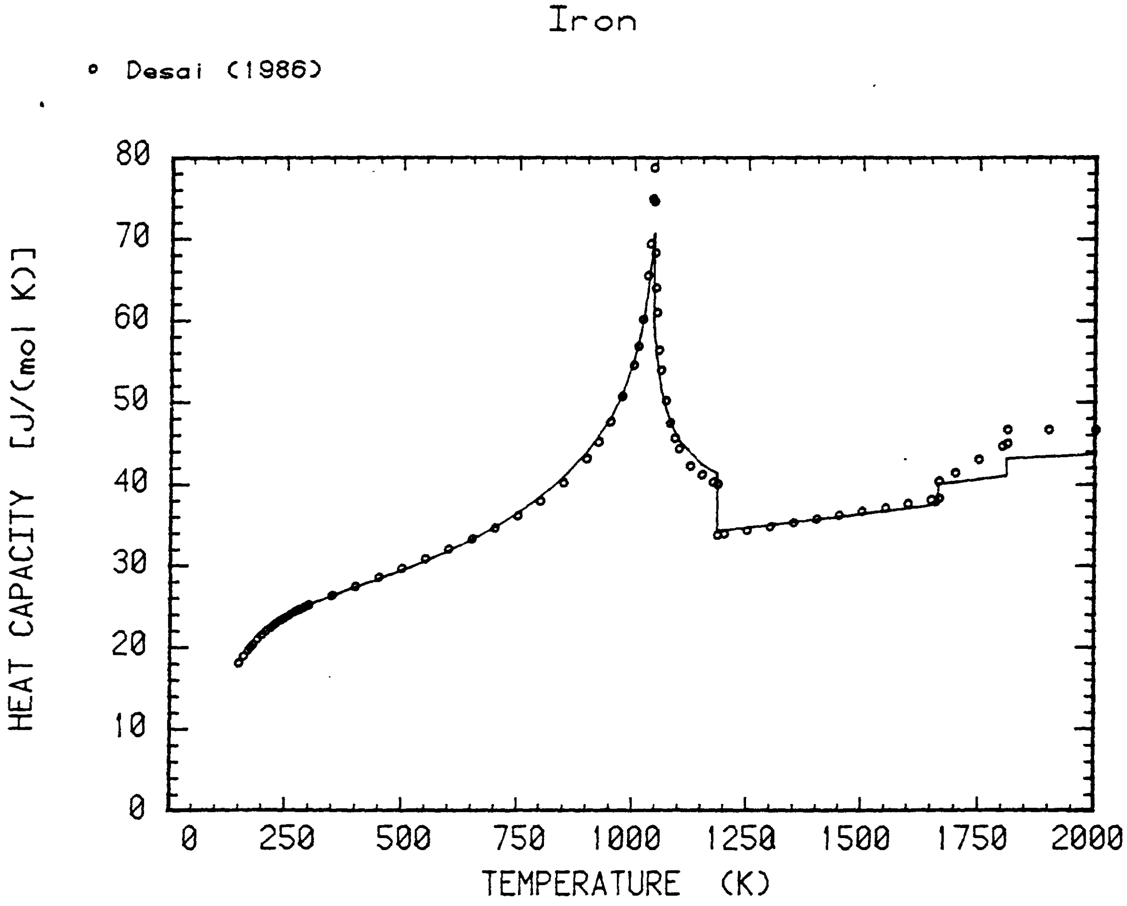


Figure 10. Comparison of the calculated heat capacities with the estimates for Fe(bcc), Fe(fcc), and Fe(liq) as reported by Desai (1986). The solid line shows the calculated heat capacity for the stable phases.

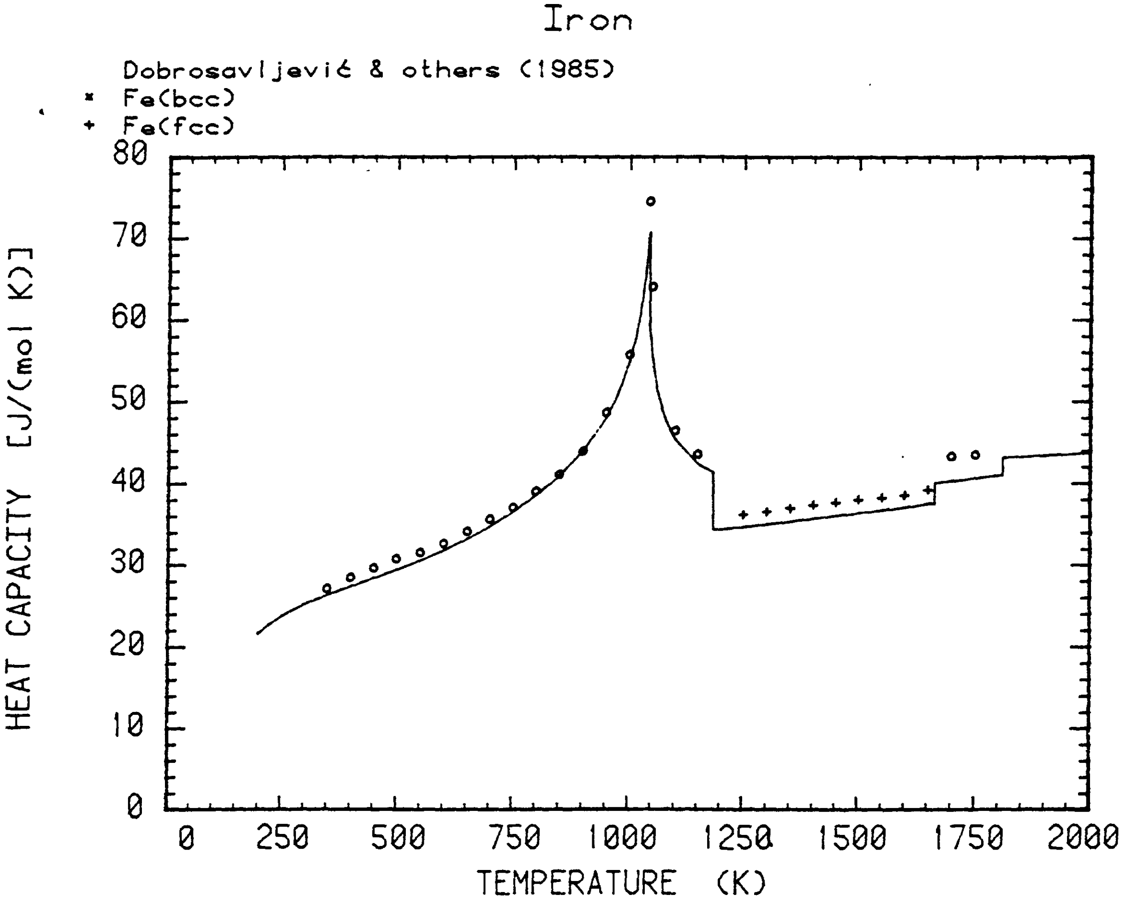


Figure 11. Comparison of the calculated heat capacities with the experimental data for Fe(bcc) and Fe(fcc) as reported by Dobrosavljević and others (1985). The solid line shows the calculated heat capacity for the stable phases.

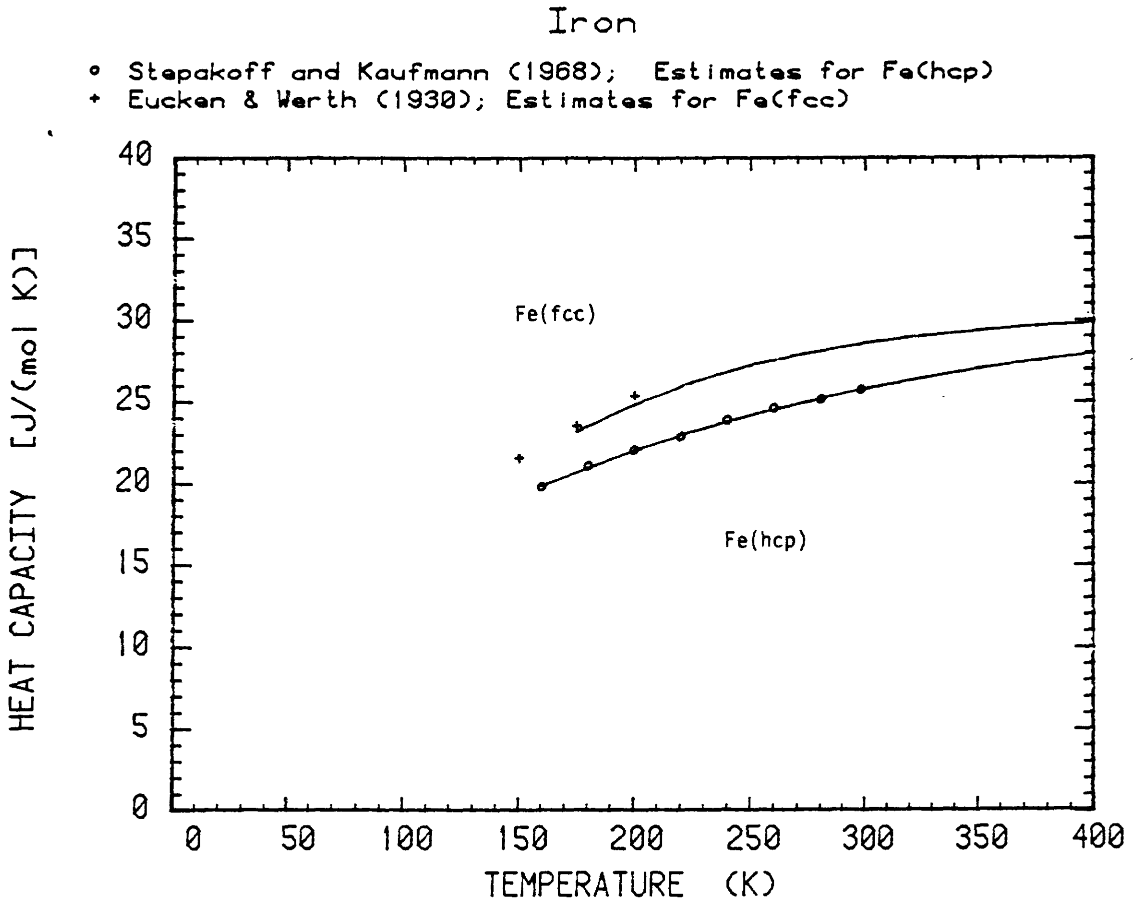


Figure 12. Comparison of the calculated heat capacities with the derived data for Fe(fcc) as reported by Eucken and Werth (1930) and of Fe(hcp) as reported by Stepakoff and Kaufman (1968) from analysis of alloys. The solid lines are the calculated values.

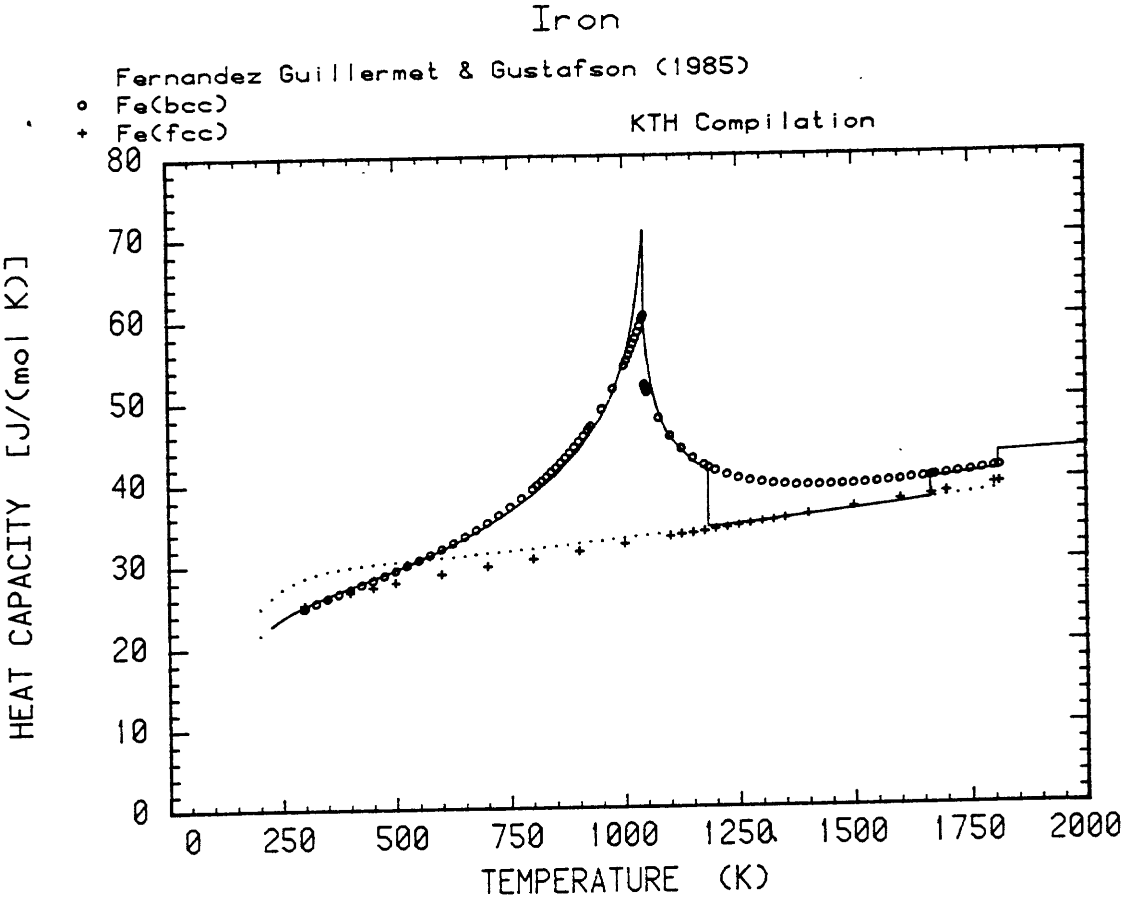


Figure 13. Comparison of the calculated heat capacities with the estimates for Fe(bcc) and Fe(fcc) as reported by Fernandez Guillermet and Gustafson (1985). The solid line shows the calculated heat capacity for the stable phases. The dotted lines are the metastable extensions of the heat capacity for Fe(fcc).

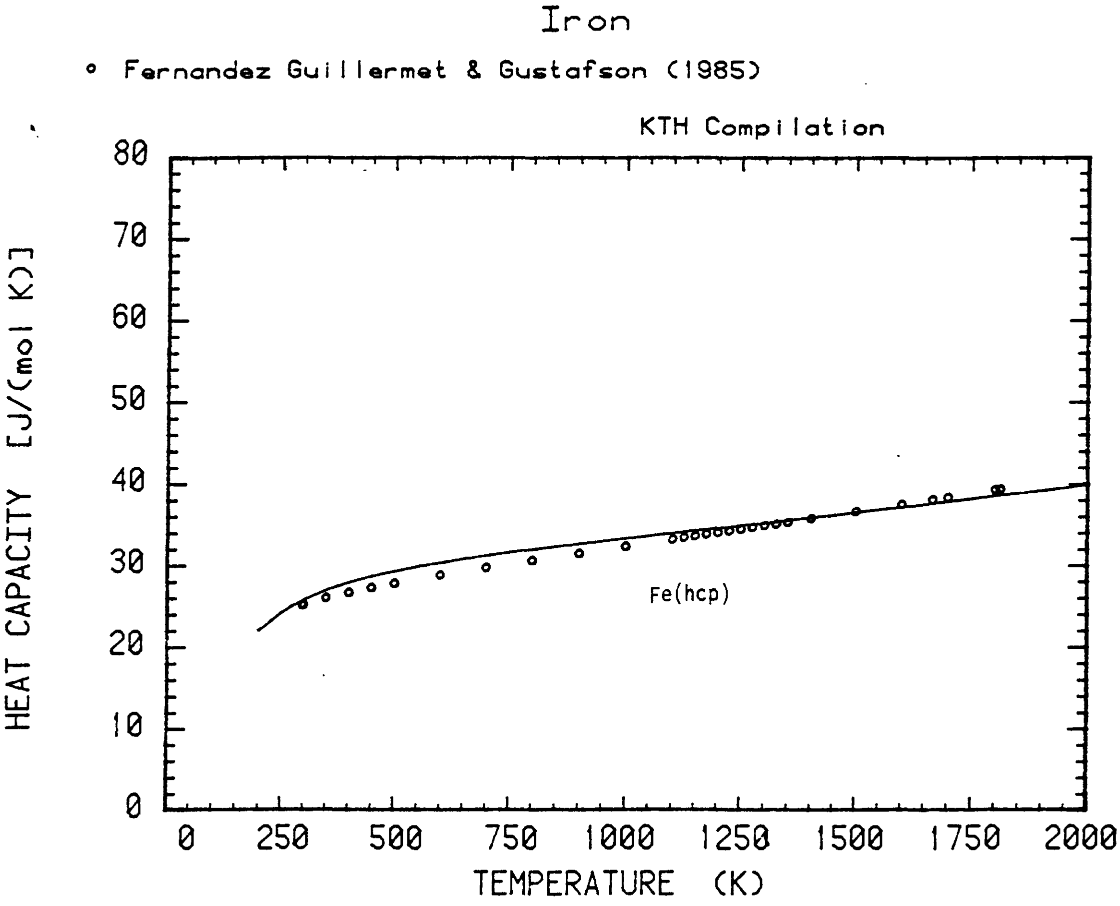


Figure 14. Comparison of the calculated heat capacities with the estimates for Fe(hcp) as reported by Fernandez Guillermet and Gustafson (1985). The solid line was calculated from equation 2 and the constants on Table 1.

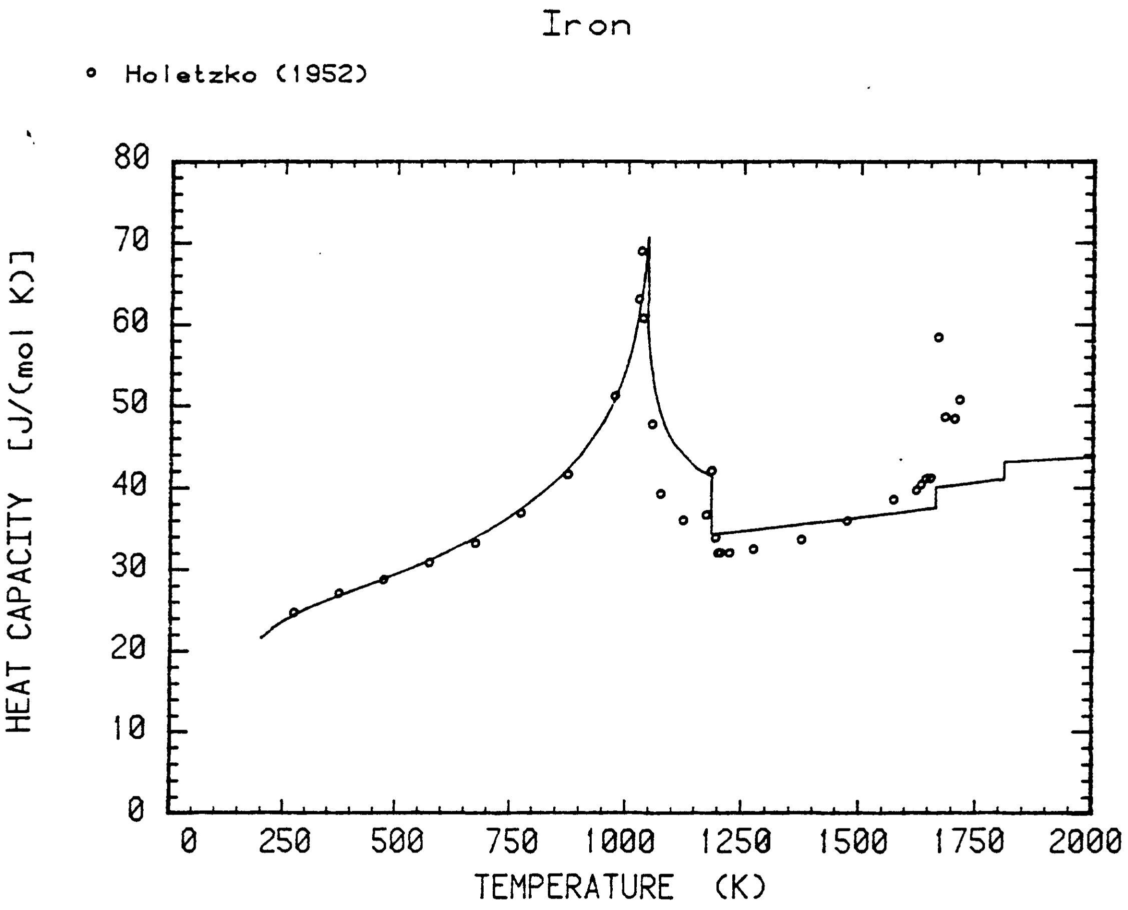


Figure 15. Comparison of the calculated heat capacities with the experimental data for Fe(bcc) and Fe(fcc) as reported by Holetzko (1950). The solid line shows the calculated heat capacity for the stable phases.

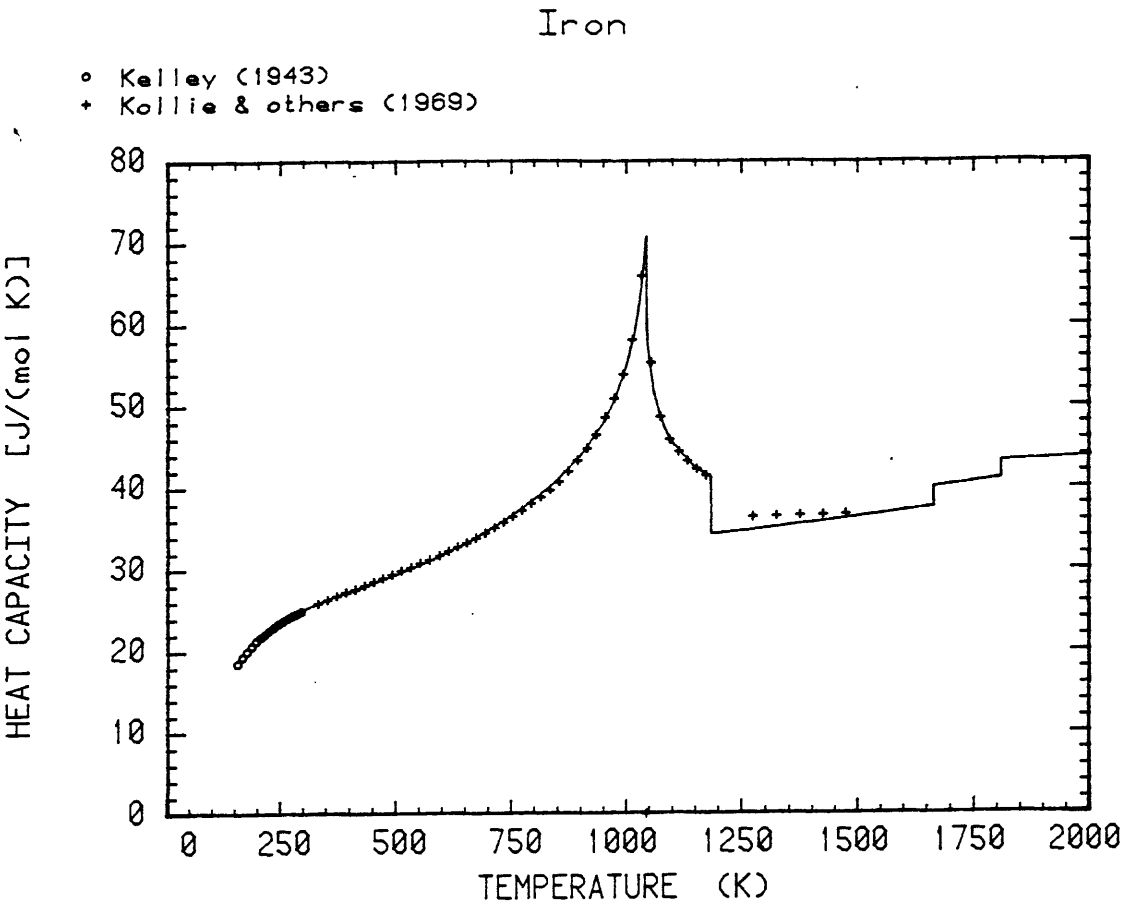


Figure 16. Comparison of the calculated heat capacities with the experimental data for Fe(bcc) as reported by Kelley (1943) and for Fe(bcc) and Fe(fcc) as reported by Kollie (1969). The solid line shows the calculated heat capacity for the stable phases.

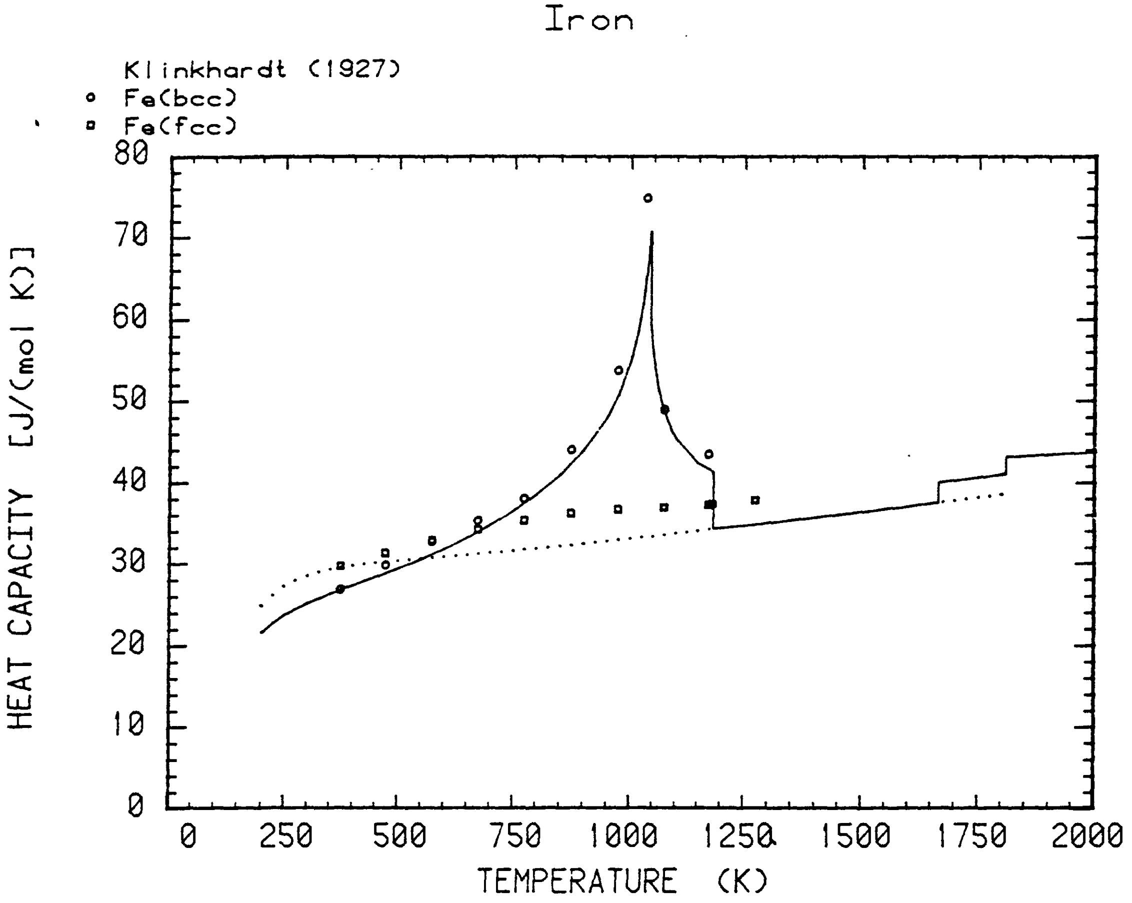


Figure 17. Comparison of the calculated heat capacities with the experimental data and estimates for Fe(bcc) and Fe(fcc) as reported by Klinkhardt (1927). The solid line shows the calculated heat capacity for the stable phases. The dotted lines are the metastable extensions of the heat capacity for Fe(fcc).

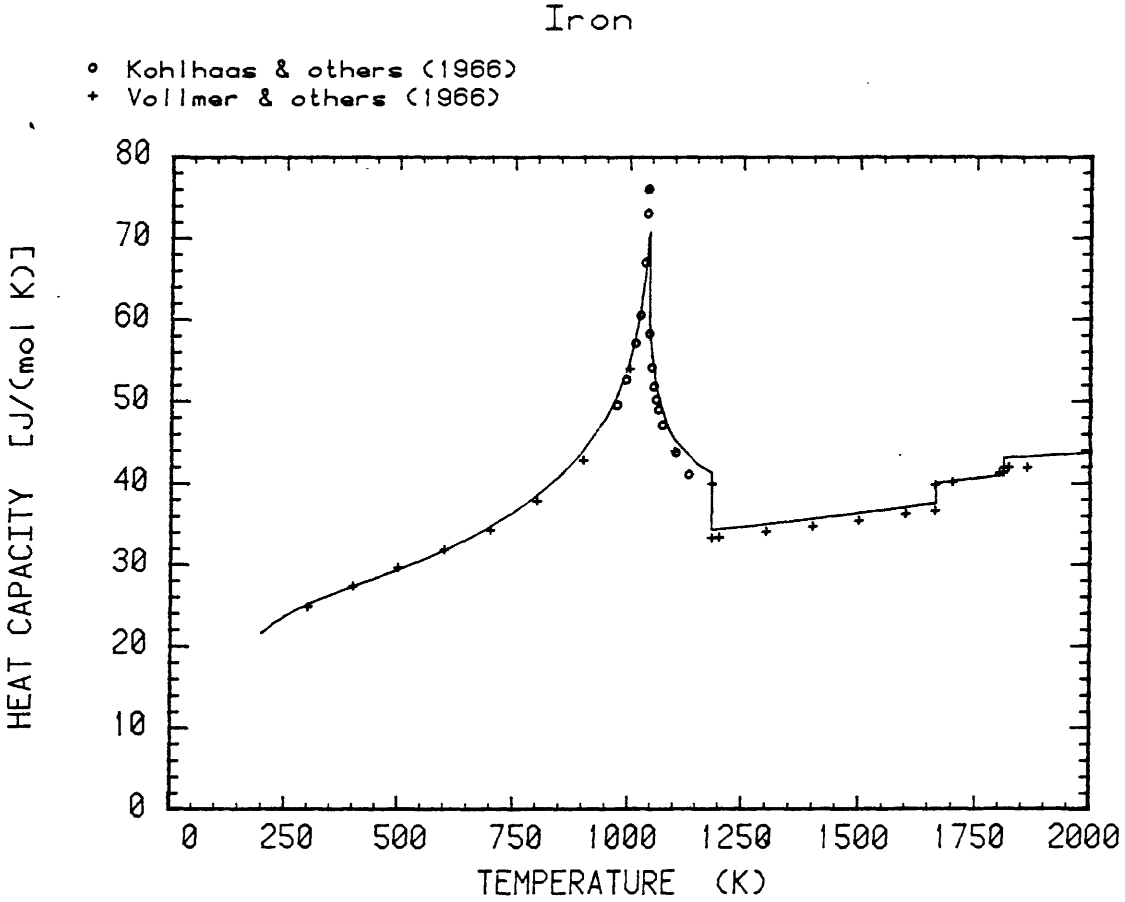


Figure 18. Comparison of the calculated heat capacities with the experimental data for Fe(bcc) as reported by Kohlhaas and others (1966) and by Vollmer and others (1966). The solid line shows the calculated heat capacity for the stable phases.

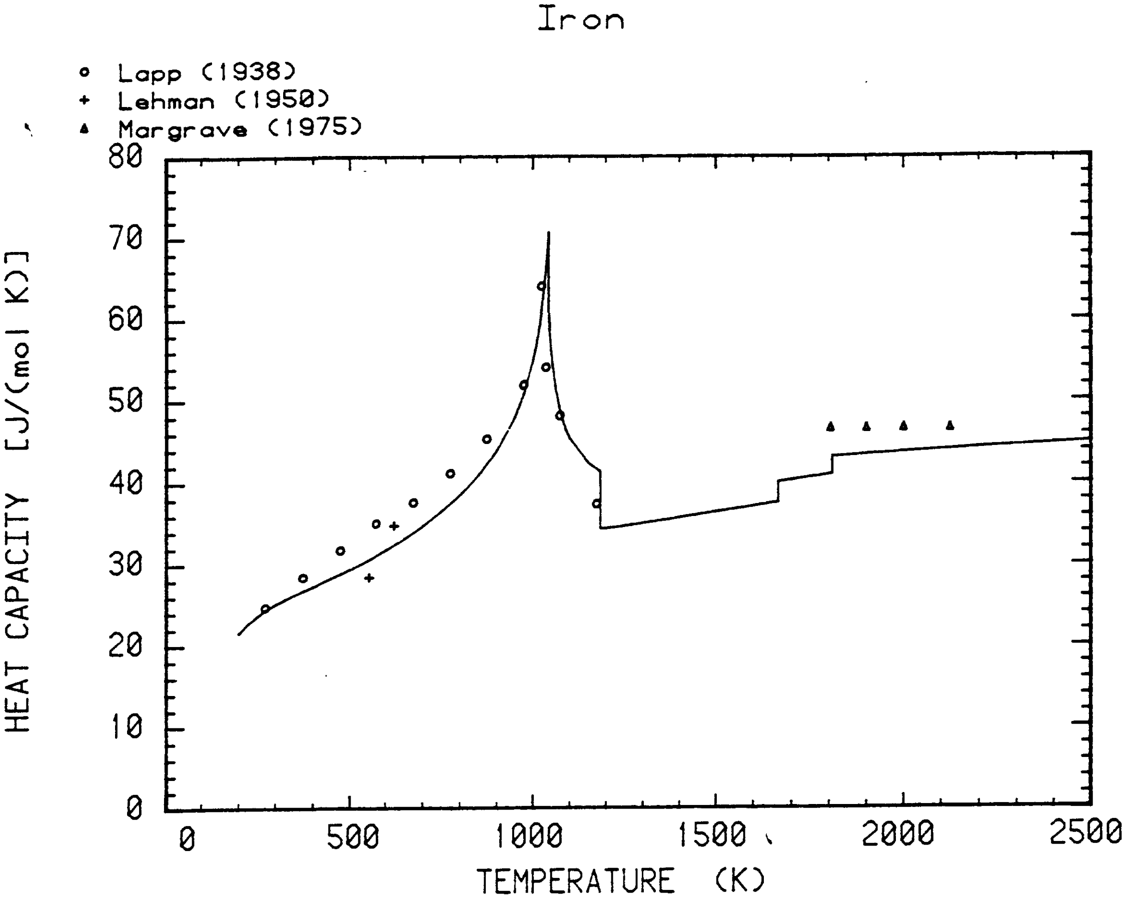


Figure 19. Comparison of the calculated heat capacities with the experimental data for Fe(bcc) and Fe(fcc) as reported by Lapp (1938), of Fe(bcc) as reported by Lehman, and of Fe(liq) as reported by Margrave (1975). The solid line shows the calculated heat capacity for the stable phases.

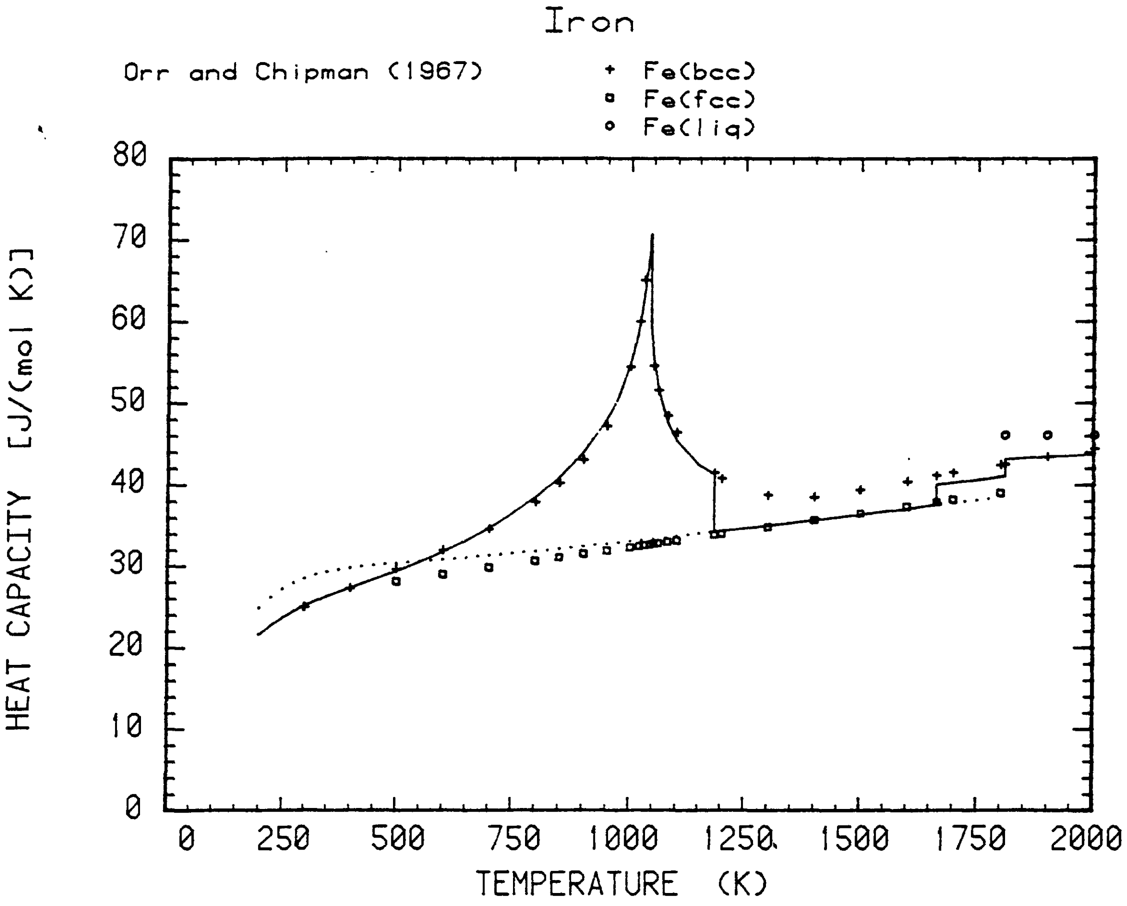


Figure 20. Comparison of the calculated heat capacities with the estimates for Fe(bcc), Fe(fcc), and Fe(liq) as reported by Orr and Chipman (1967). The solid line shows the calculated heat capacity for the stable phases. The dotted lines are the metastable extensions of the heat capacity for Fe(fcc).

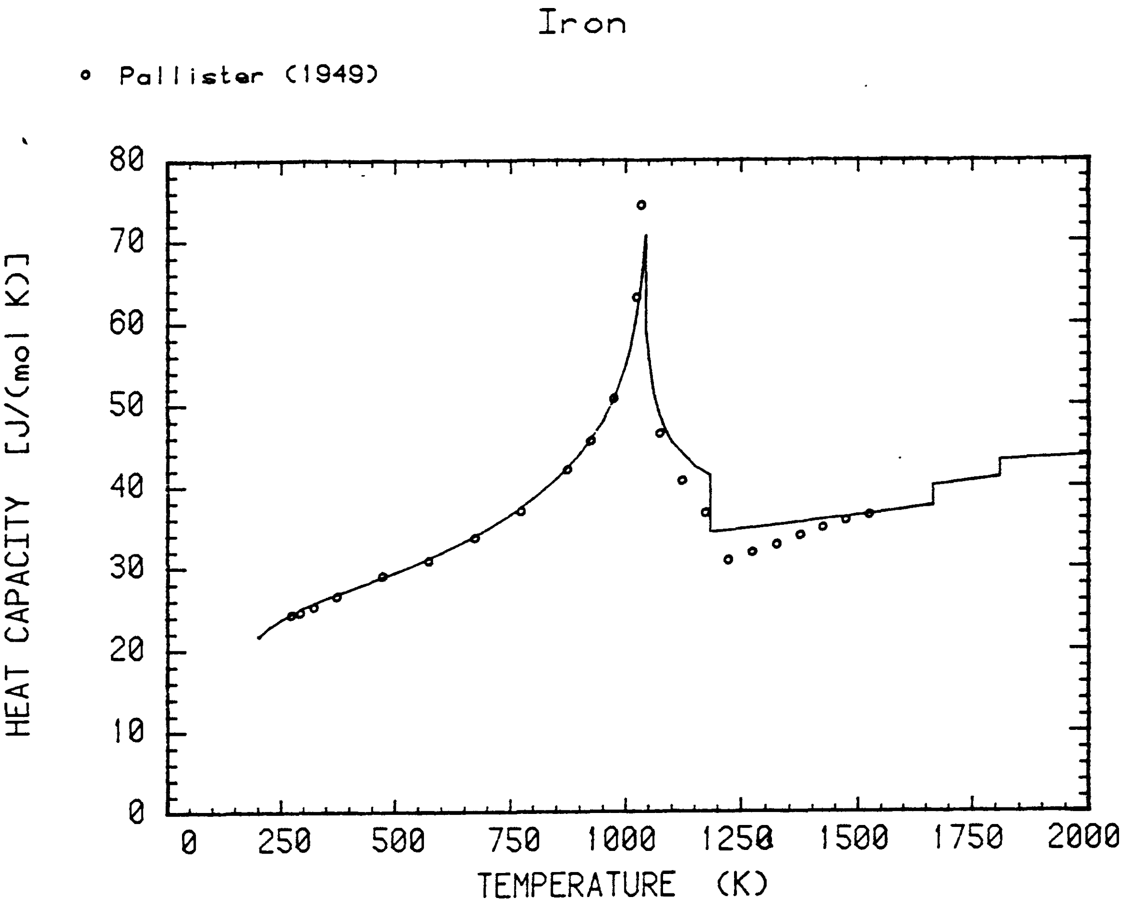


Figure 21. Comparison of the calculated heat capacities with the experimental data for Fe(bcc) and Fe(fcc) as reported by Pallister (1949). The solid line shows the calculated heat capacity for the stable phases.

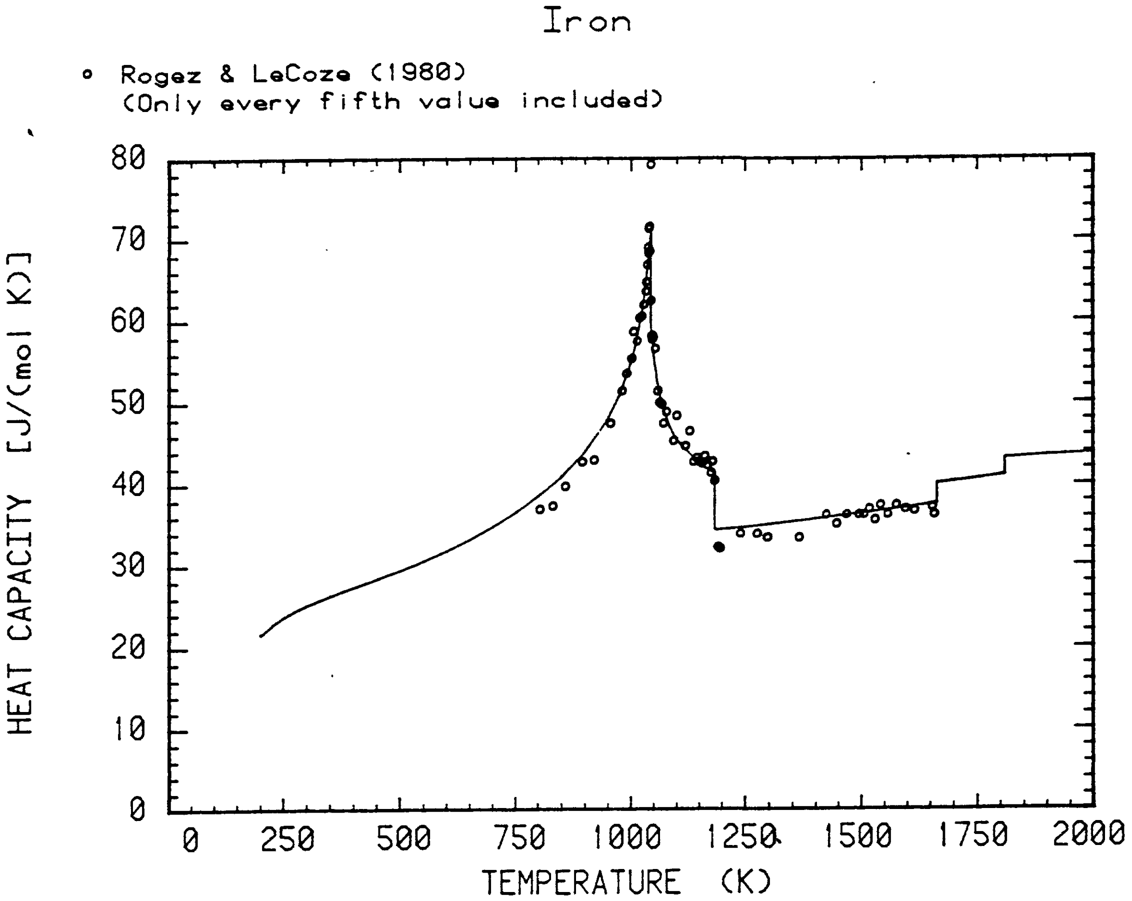


Figure 22. Comparison of the calculated heat capacities with the experimental data for Fe(bcc) and Fe(fcc) as reported by Rogez and LeCoze (1980). The solid line shows the calculated heat capacity for the stable phases.

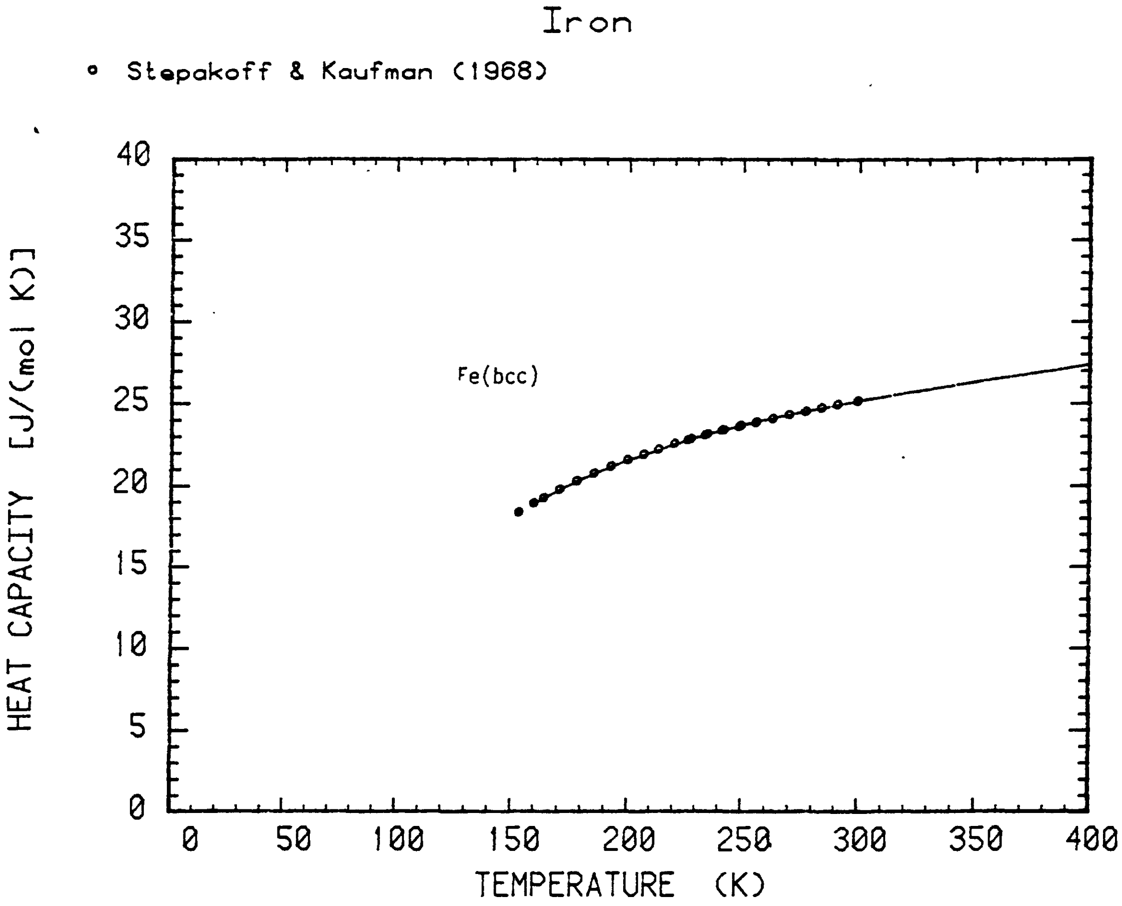


Figure 23. Comparison of the calculated heat capacities with the experimental data for Fe(bcc) as reported by Stepakoff and Kaufman (1968). The solid line shows the calculated heat capacity for Fe(bcc).

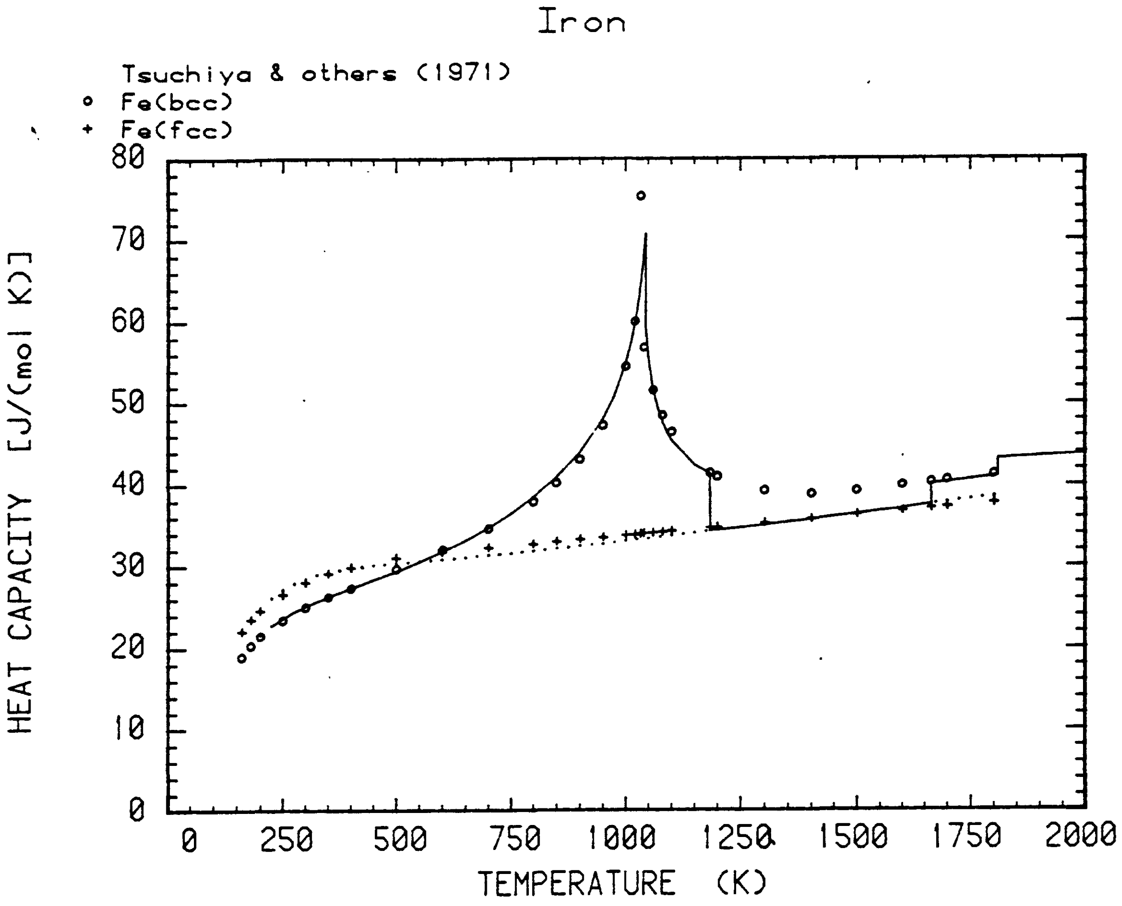


Figure 24. Comparison of the calculated heat capacities with the experimental data and estimates for Fe(bcc) and Fe(fcc) as reported by Tsuchiya and others (1971). The solid line shows the calculated heat capacity for the stable phases. The dotted lines are the metastable extensions of the heat capacity for Fe(fcc).

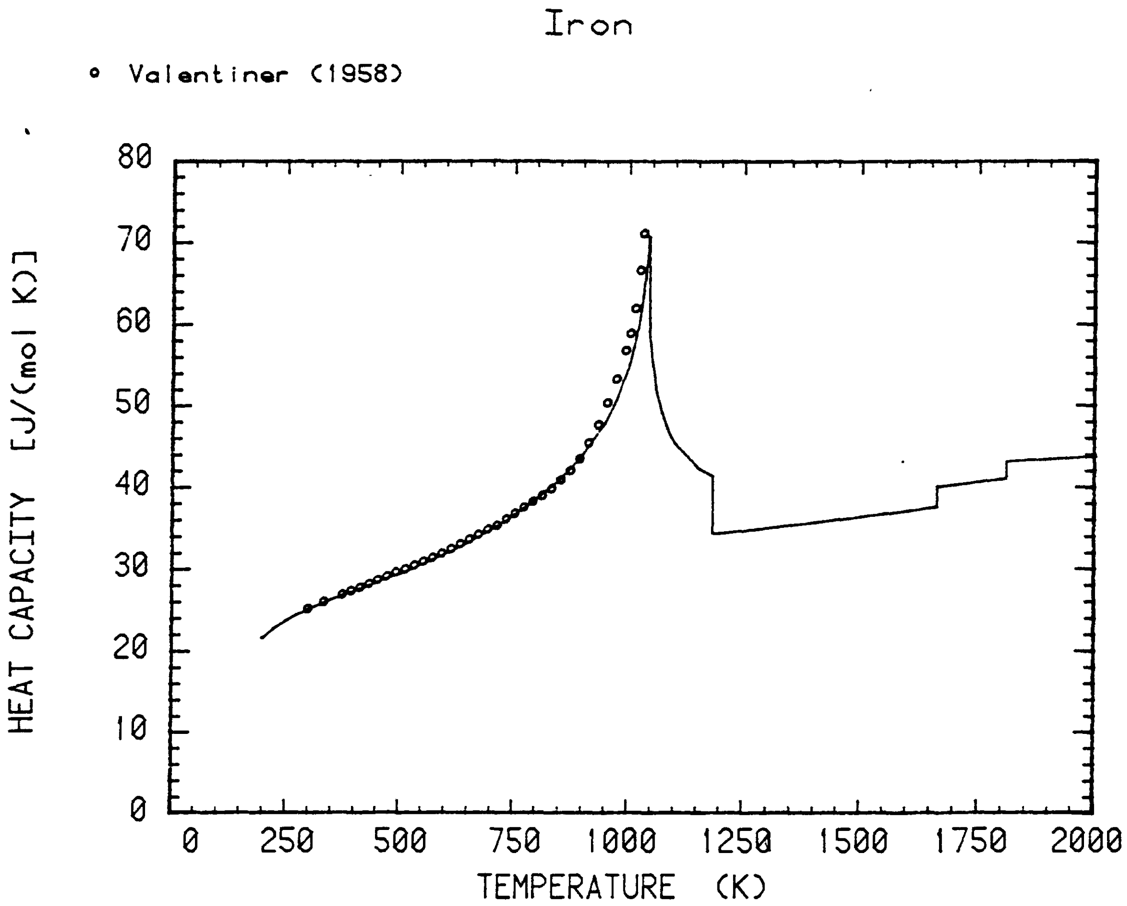


Figure 25. Comparison of the calculated heat capacities with the experimental data for Fe(bcc) as reported by Valentiner (1958). The solid line shows the calculated heat capacity for Fe(bcc).

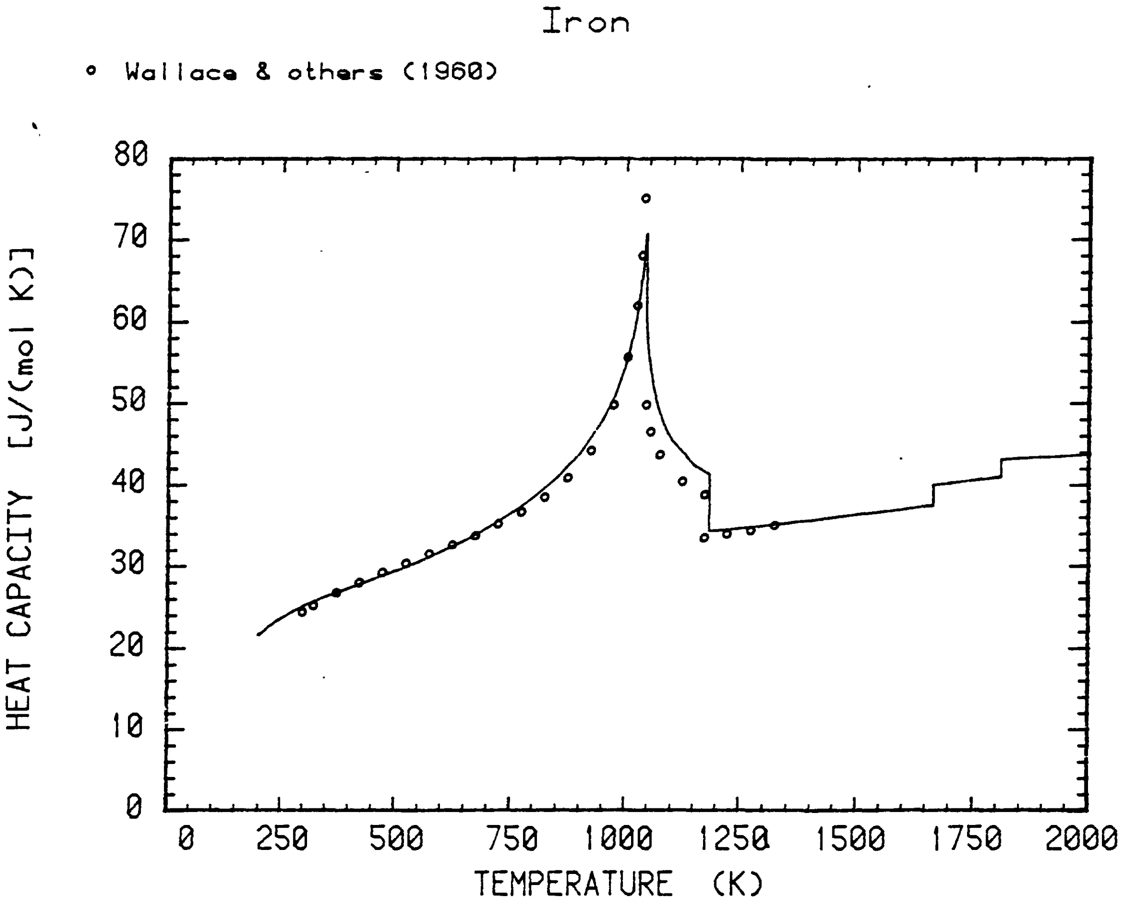


Figure 26. Comparison of the calculated heat capacities with the experimental data for Fe(bcc) and Fe(fcc) as reported by Wallace and others (1960). The solid line shows the calculated heat capacity for the stable phases.

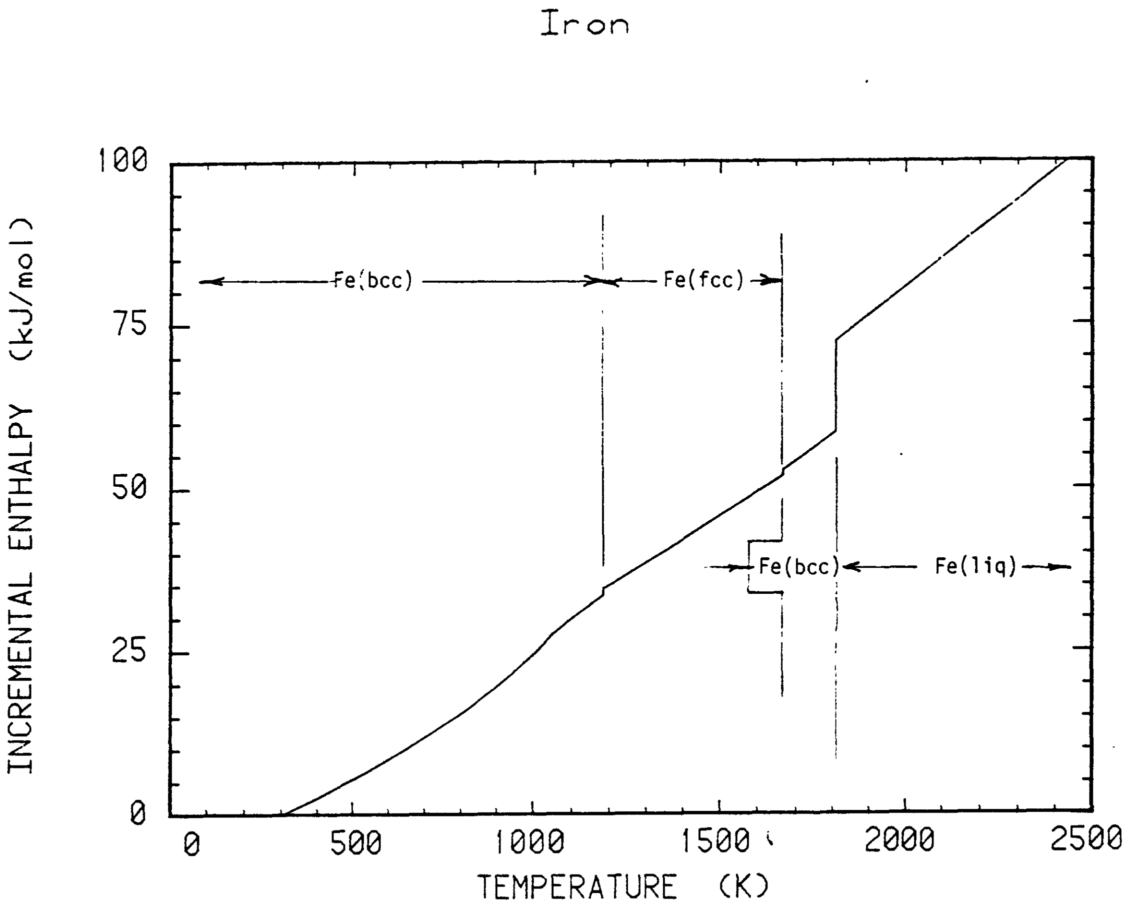


Figure 27. Calculated incremental enthalpies for the stable phases of iron.

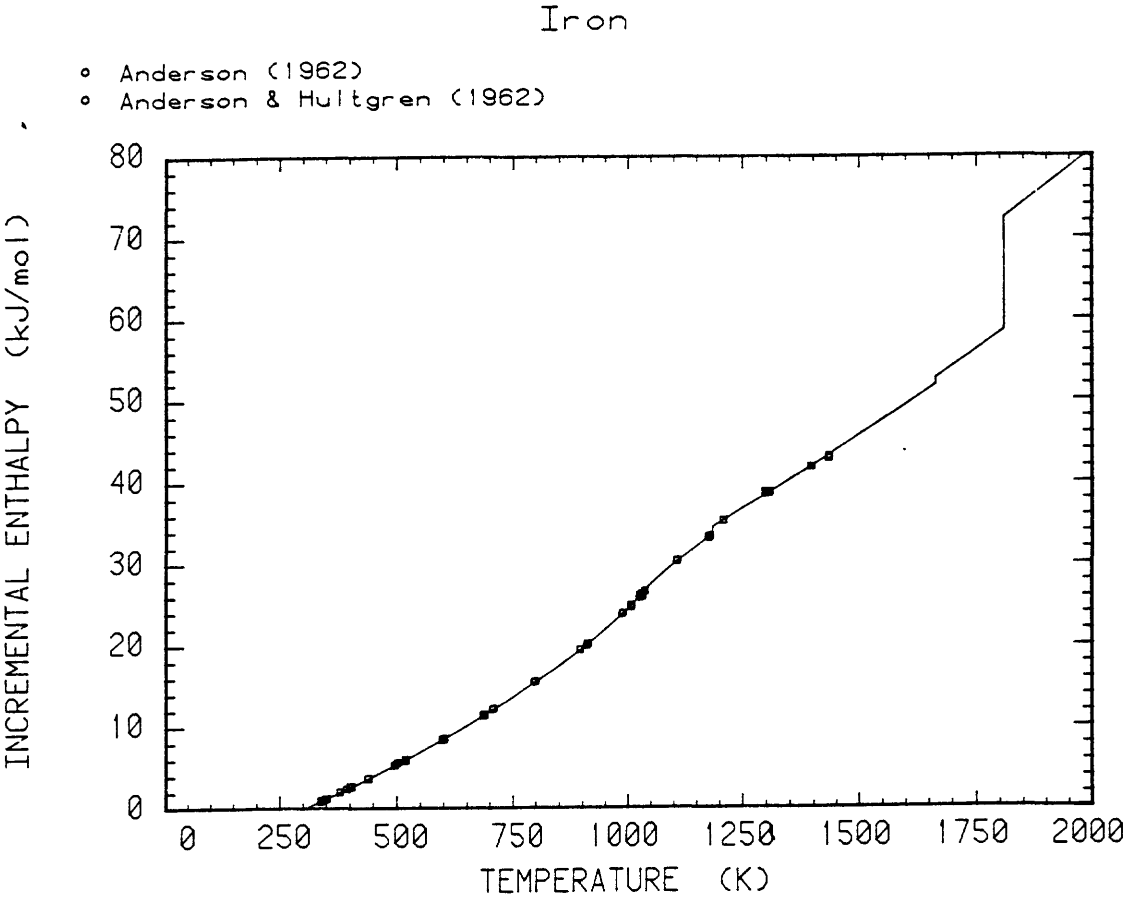


Figure 28. Comparison of calculated incremental enthalpies with the experimental data as reported by Anderson and Holtgren (1962). The solid line shows the calculated incremental enthalpies for the stable phases.

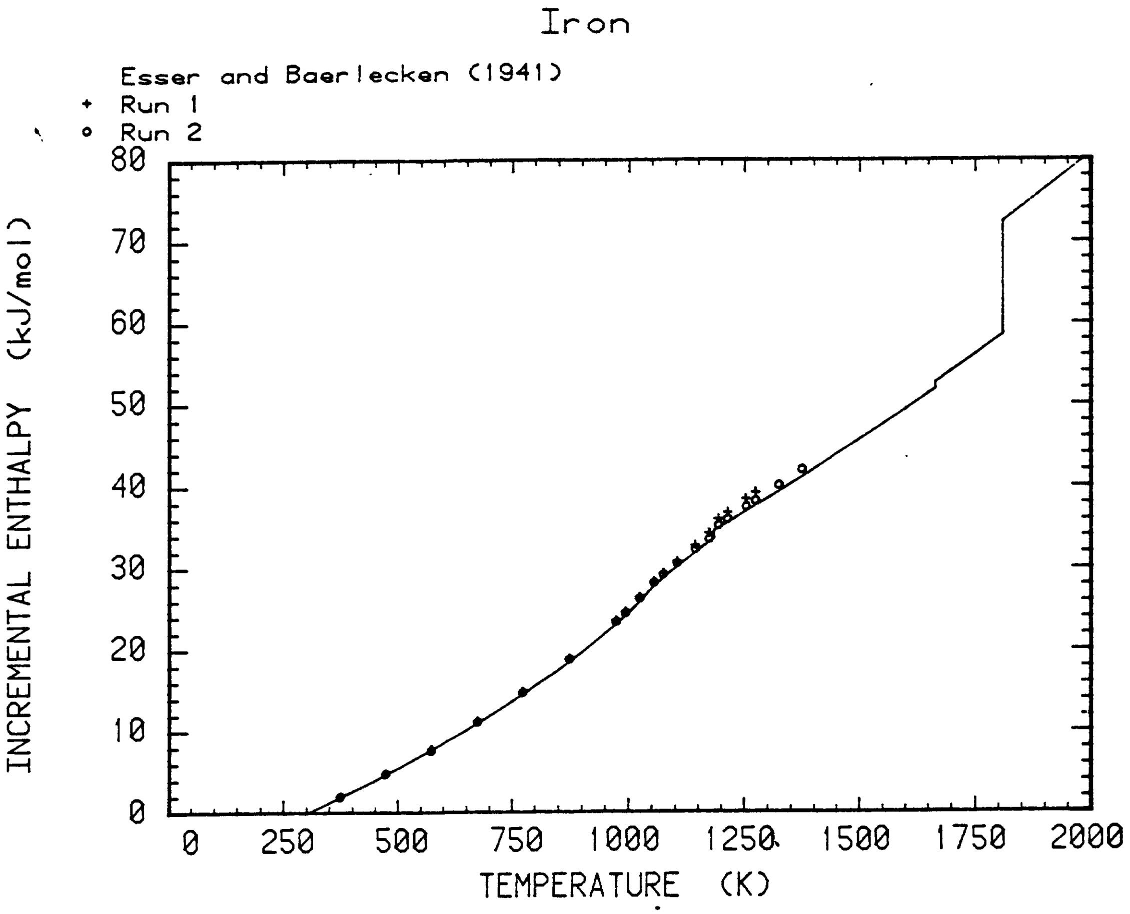


Figure 29. Comparison of the calculated incremental enthalpies with the experimental data for Fe(bcc) and Fe(fcc) as reported by Esser and Baerlecken (1941). The solid line shows the calculated incremental enthalpy for the stable phases.

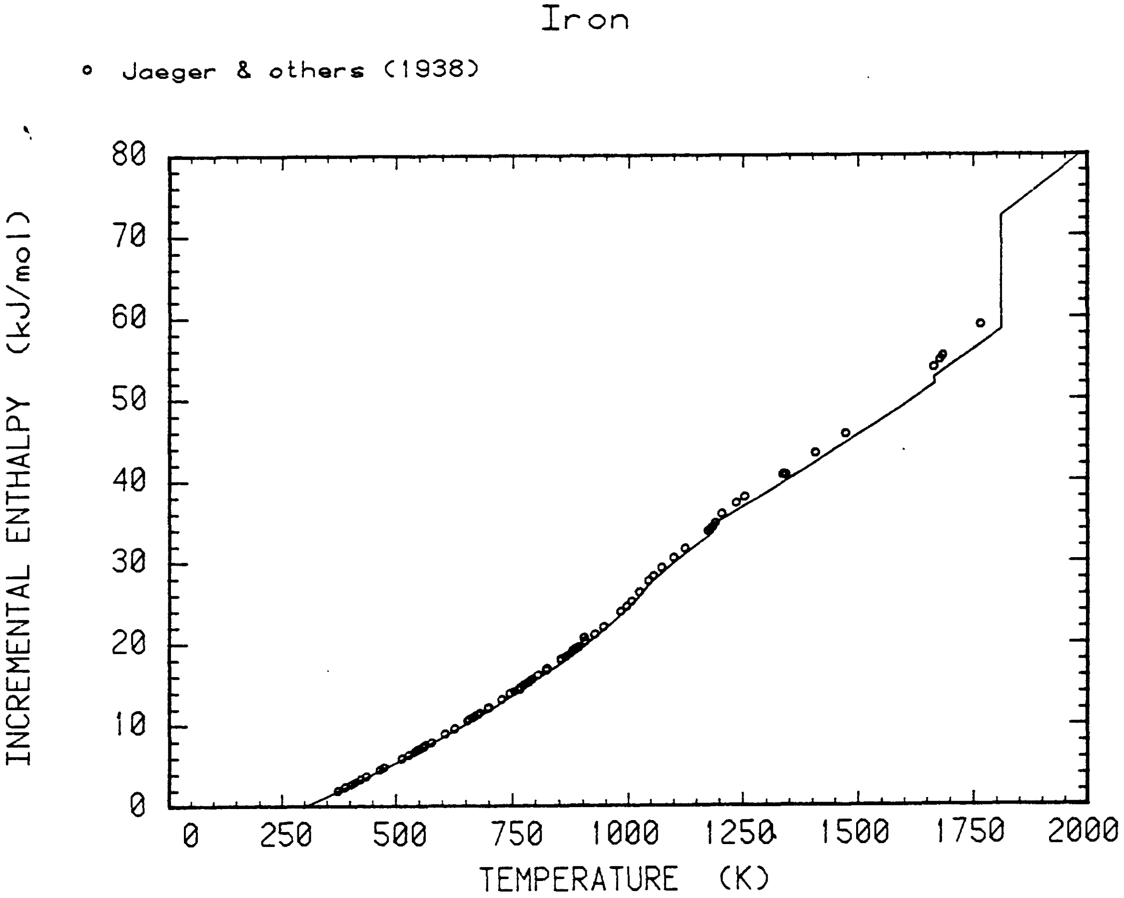


Figure 30. Comparison of calculated incremental enthalpies with the experimental data as reported by Jaeger and others (1938). The solid line shows the calculated incremental enthalpies for the stable phases.

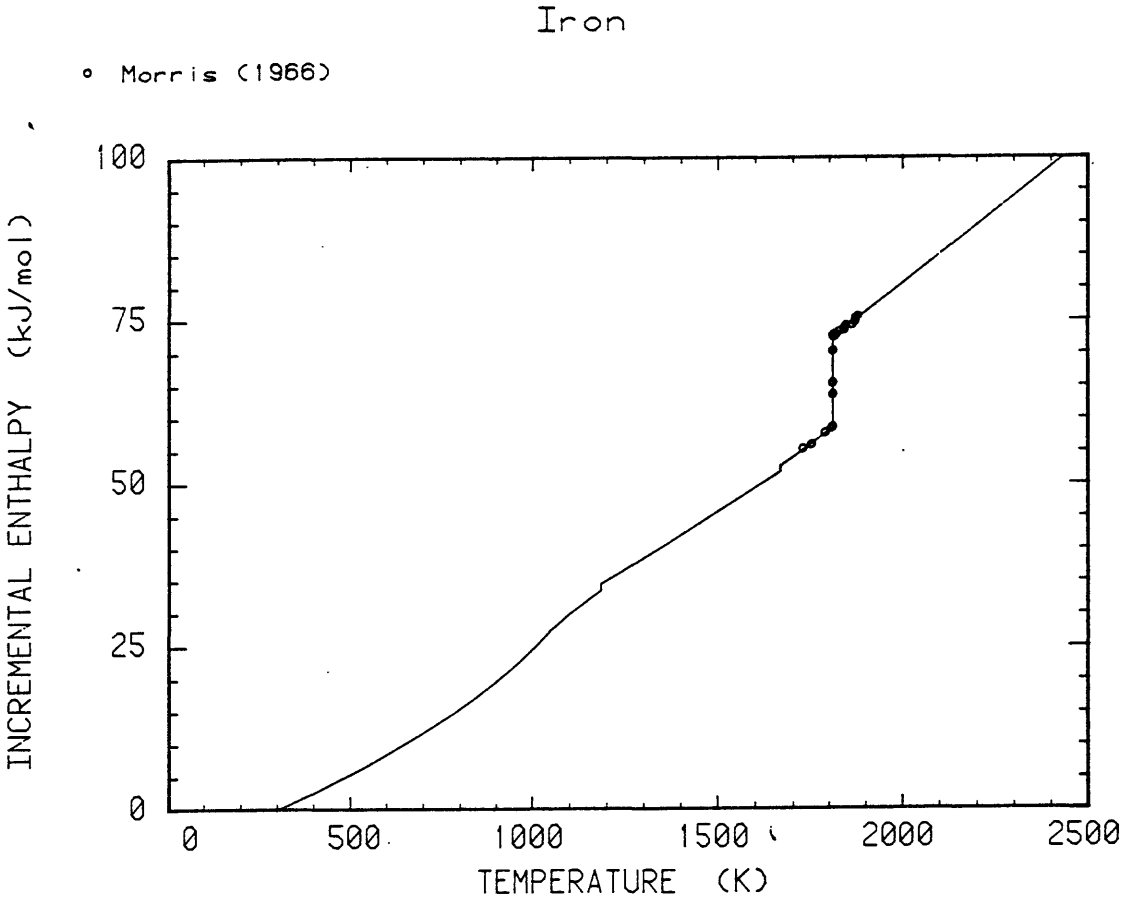


Figure 31. Comparison of calculated incremental enthalpies with the experimental data as reported by Morris (1966). The solid line shows the calculated incremental enthalpies for the stable phases.

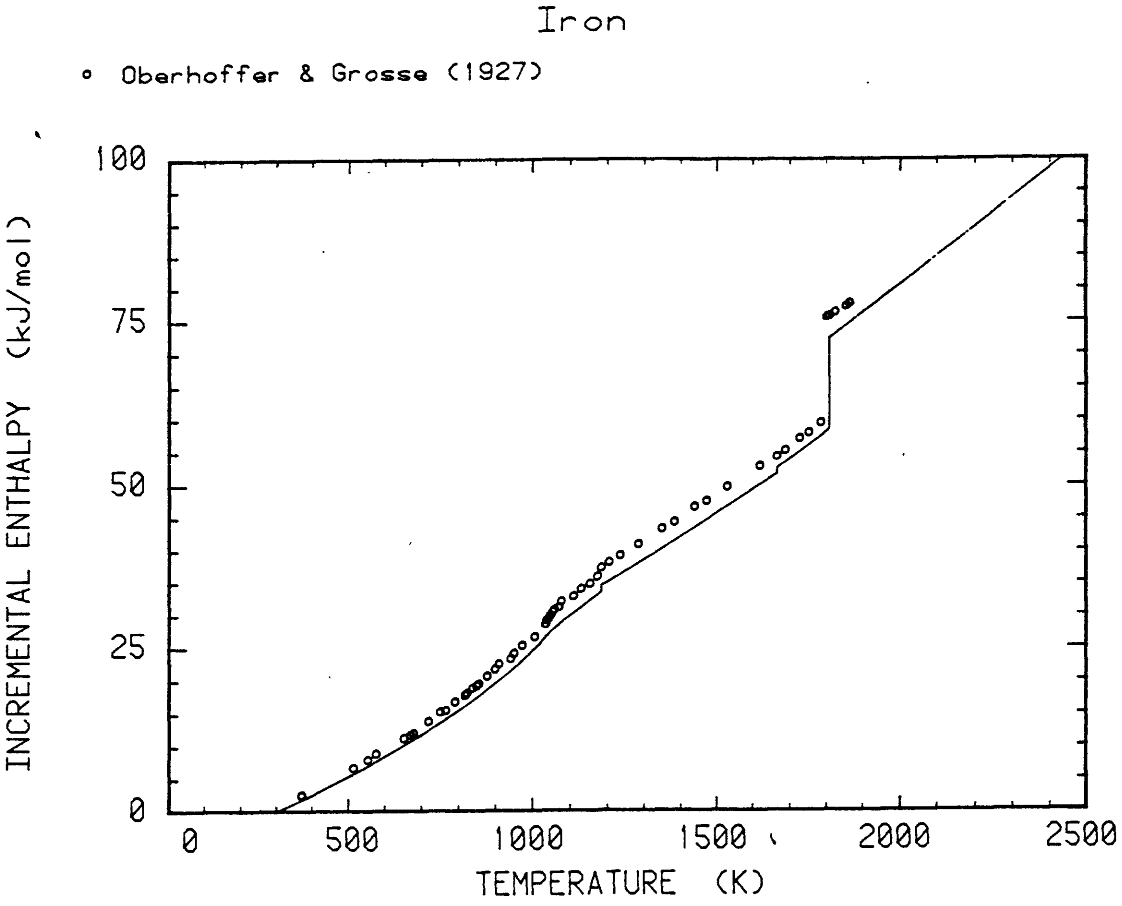


Figure 32. Comparison of calculated incremental enthalpies with the experimental data as reported by Oberhoffer and Grosse (1927). The solid line shows the calculated incremental enthalpies for the stable phases.

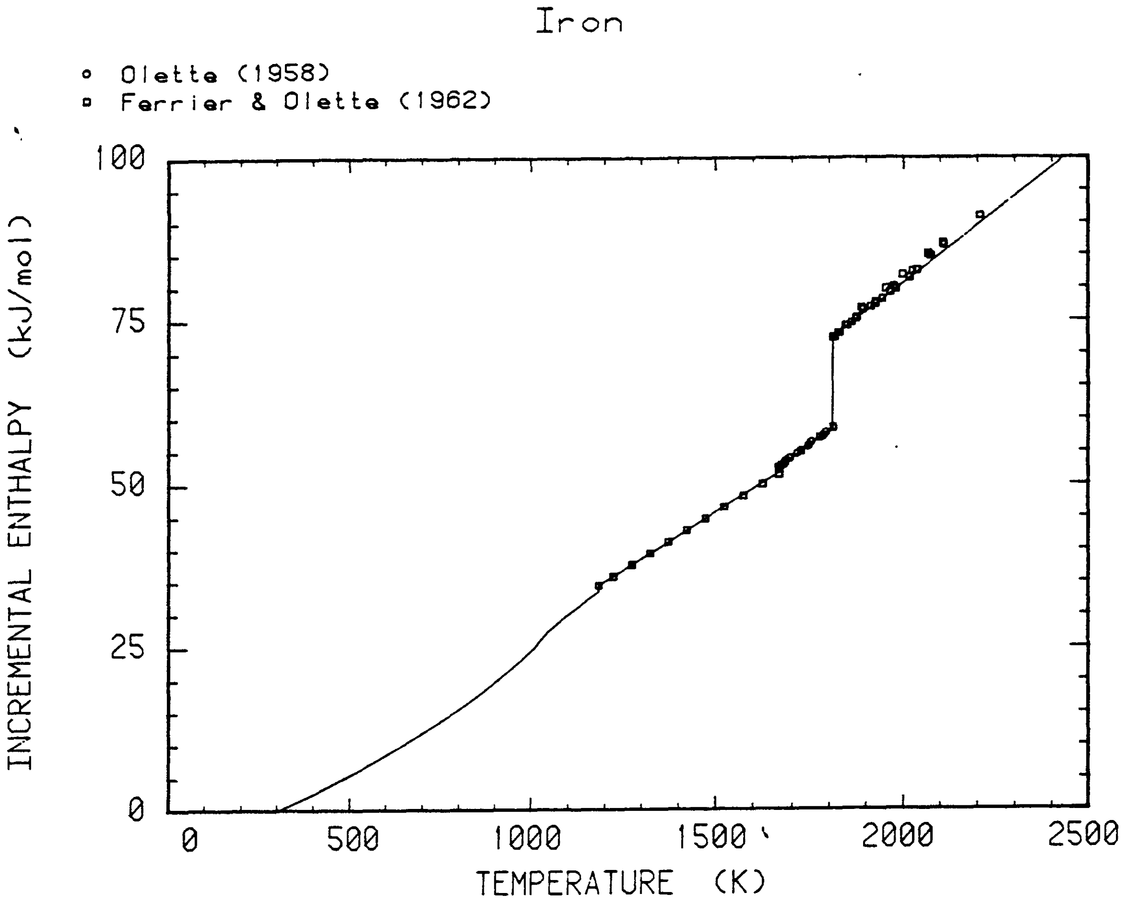


Figure 33. Comparison of calculated incremental enthalpies with the experimental data as reported by Olette (1958), Olette and Ferrier (1958), and Ferrier and Olette (1962). The solid line shows the calculated incremental enthalpies for the stable phases.

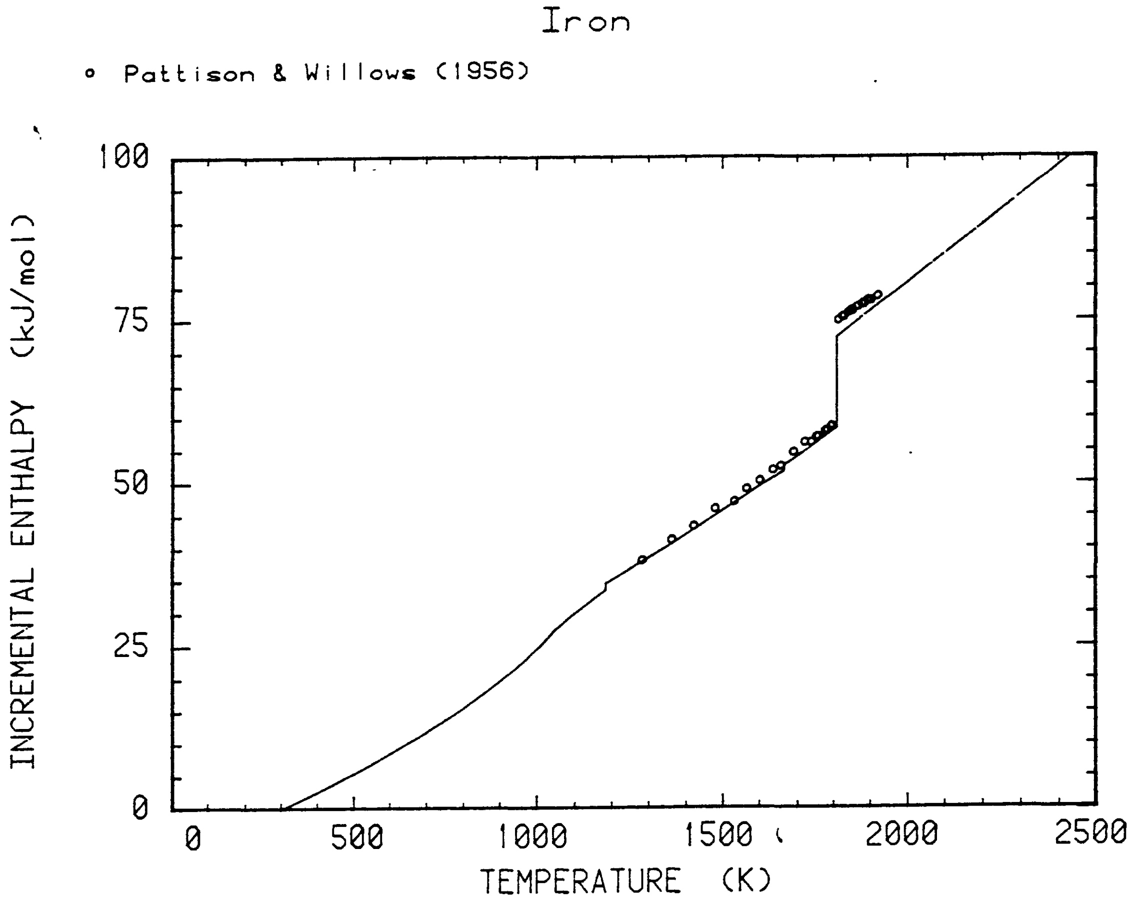


Figure 34. Comparison of calculated incremental enthalpies with the experimental data as reported by Pattison and Willows (1956). The solid line shows the calculated incremental enthalpies for the stable phases.

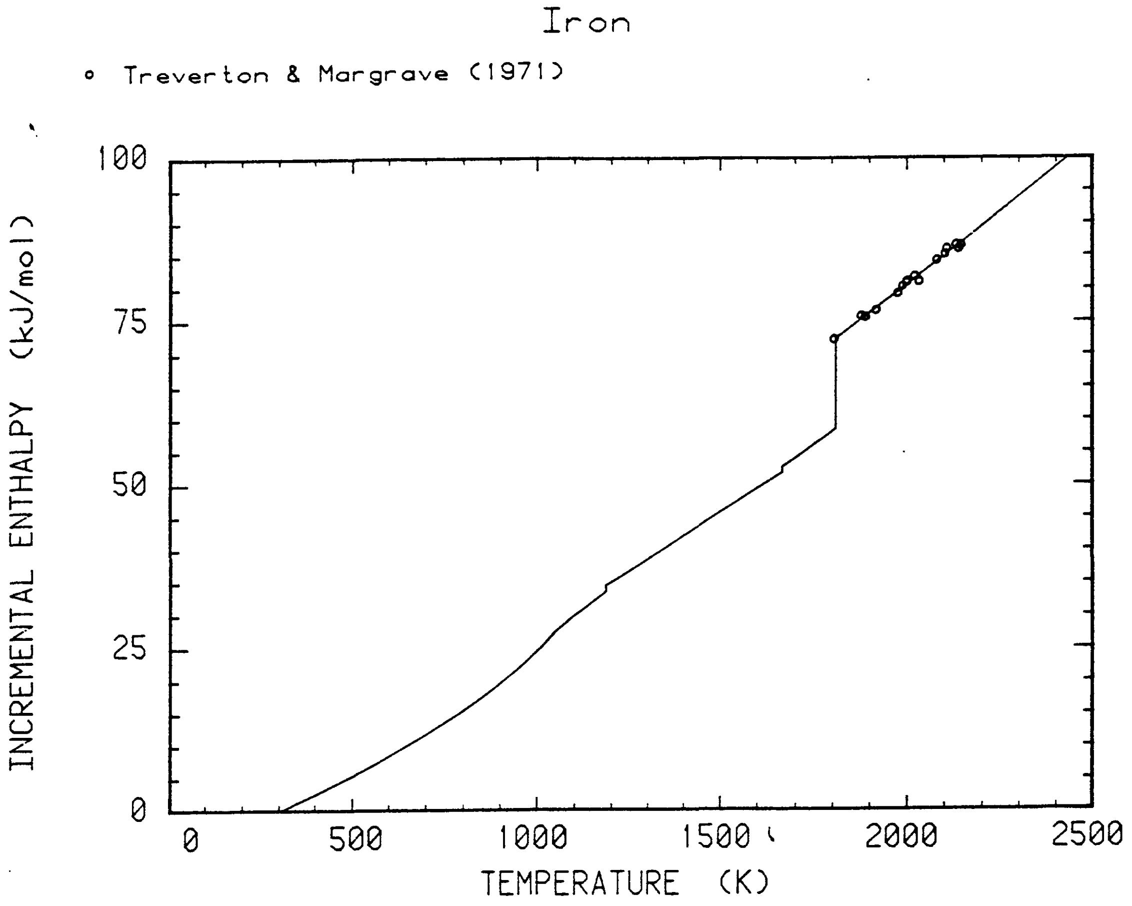


Figure 35. Comparison of calculated incremental enthalpies with the experimental data as reported by Treverton and Margrave (1971). The solid line shows the calculated incremental enthalpies for the stable phases.

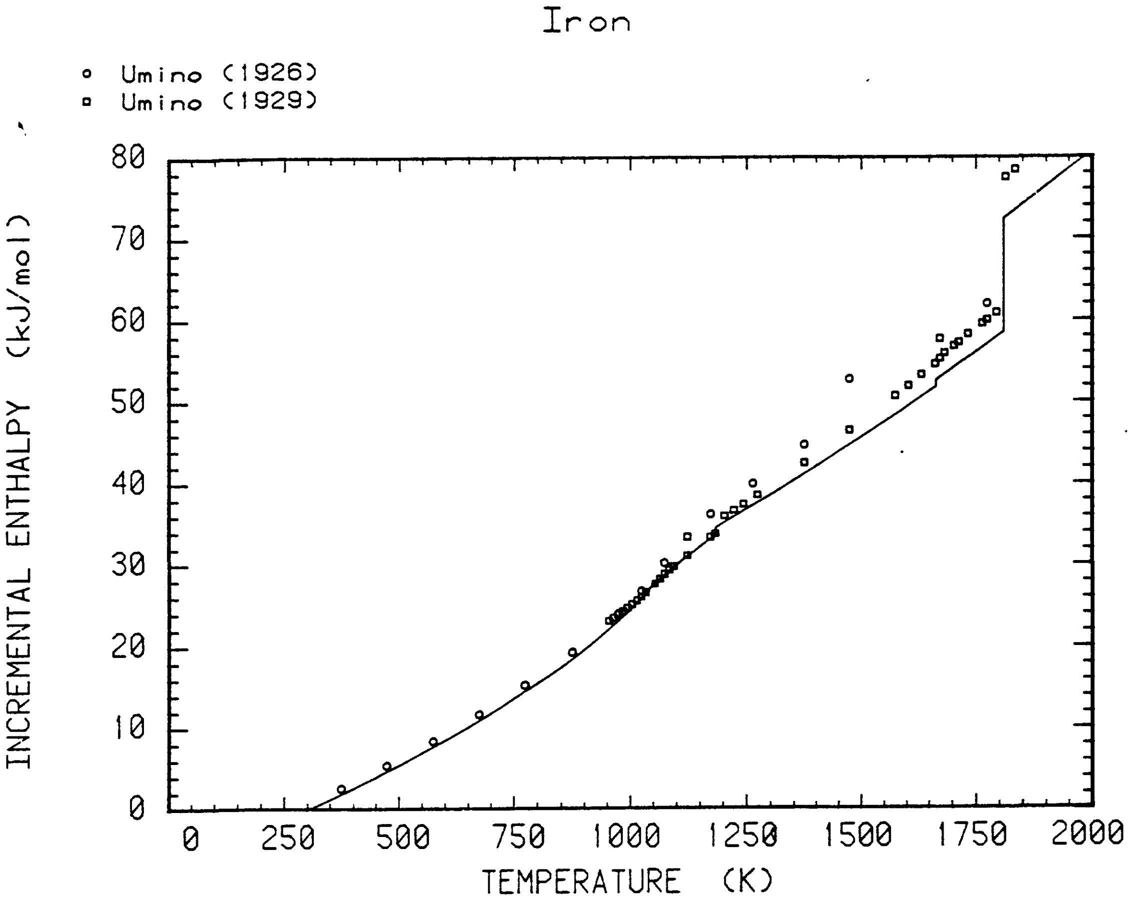


Figure 36. Comparison of calculated incremental enthalpies with the experimental data as reported by Umino (1926, 1929). The solid line shows the calculated incremental enthalpies for the stable phases.

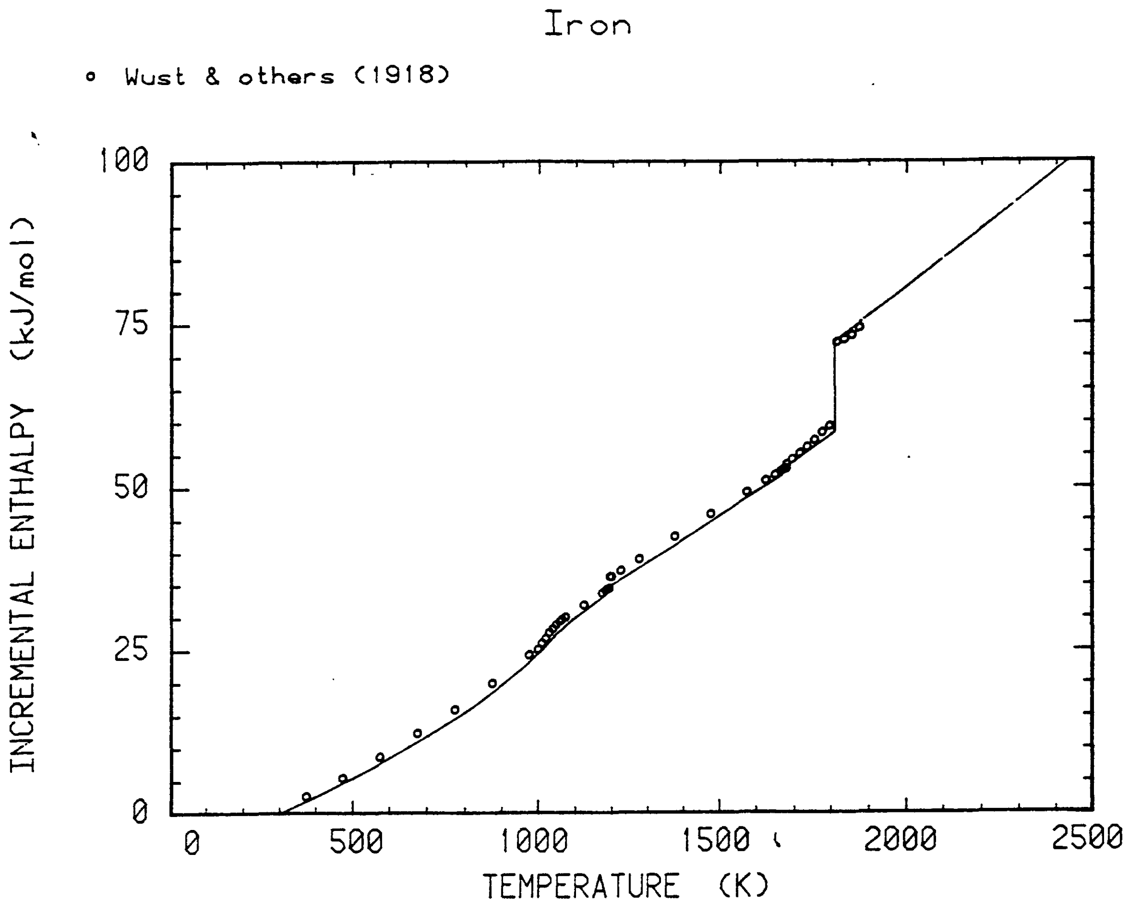


Figure 37. Comparison of calculated incremental enthalpies with the experimental data as reported by Wust and others (1918). The solid line shows the calculated incremental enthalpies for the stable phases.

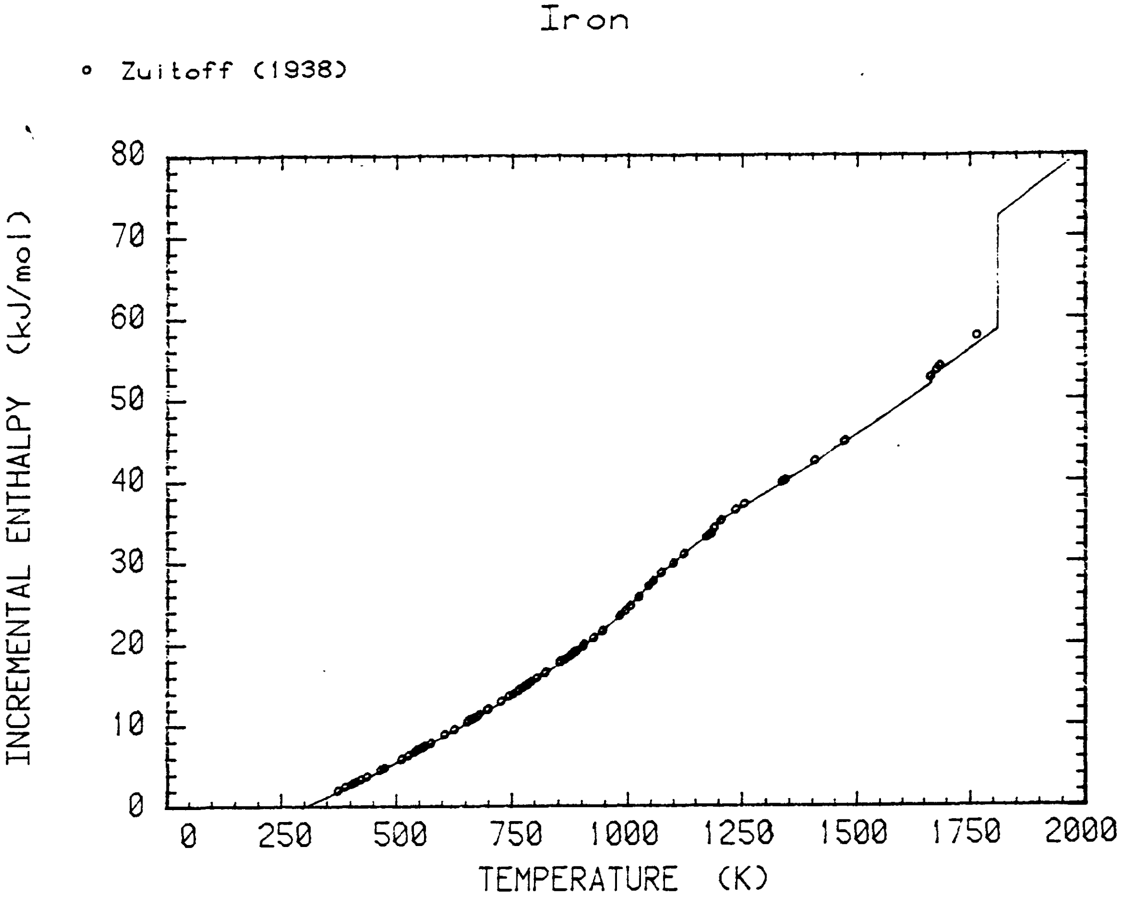


Figure 38. Comparison of calculated incremental enthalpies with the experimental data as reported by Zuitoff and others (1938).

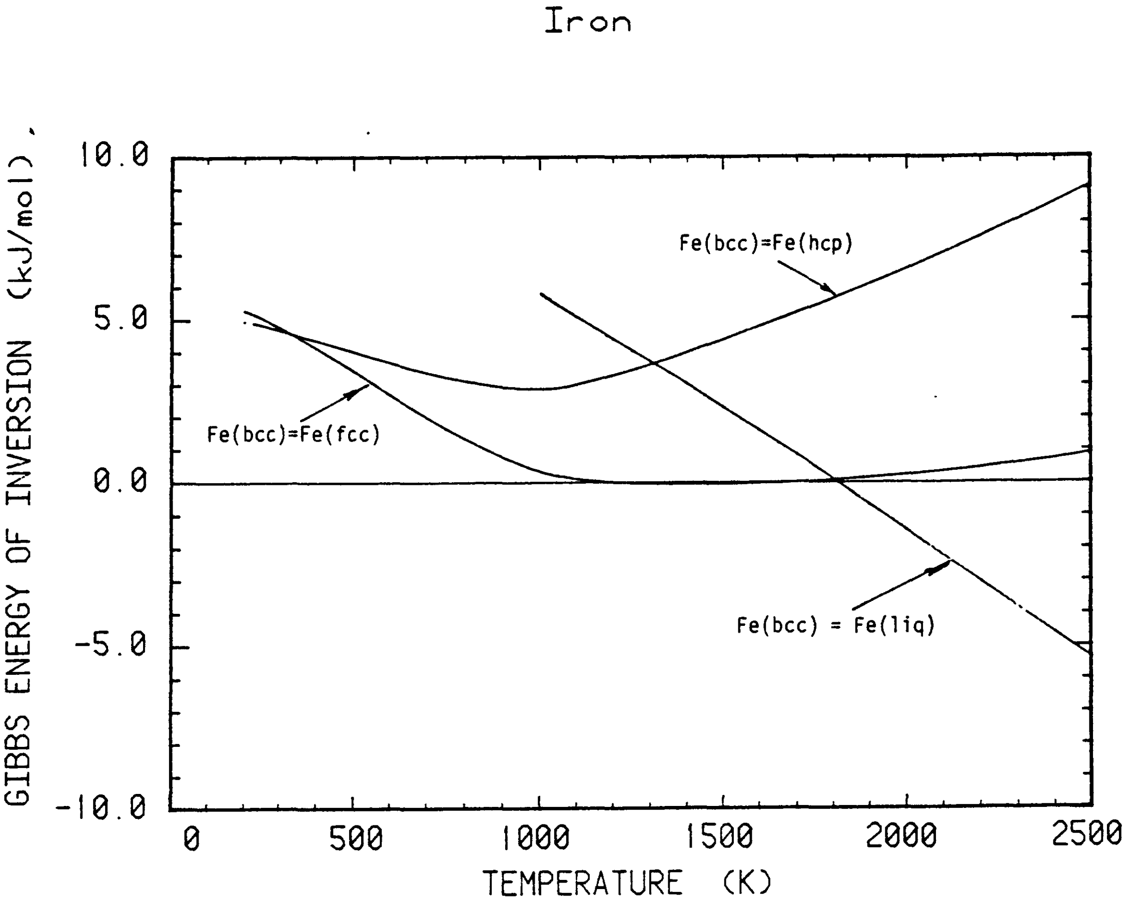


Figure 39. Plot of the calculated differences in the Gibbs energy of Fe(bcc) and the Gibbs energies of the phases Fe(fcc), Fe(hcp), and Fe(liq).

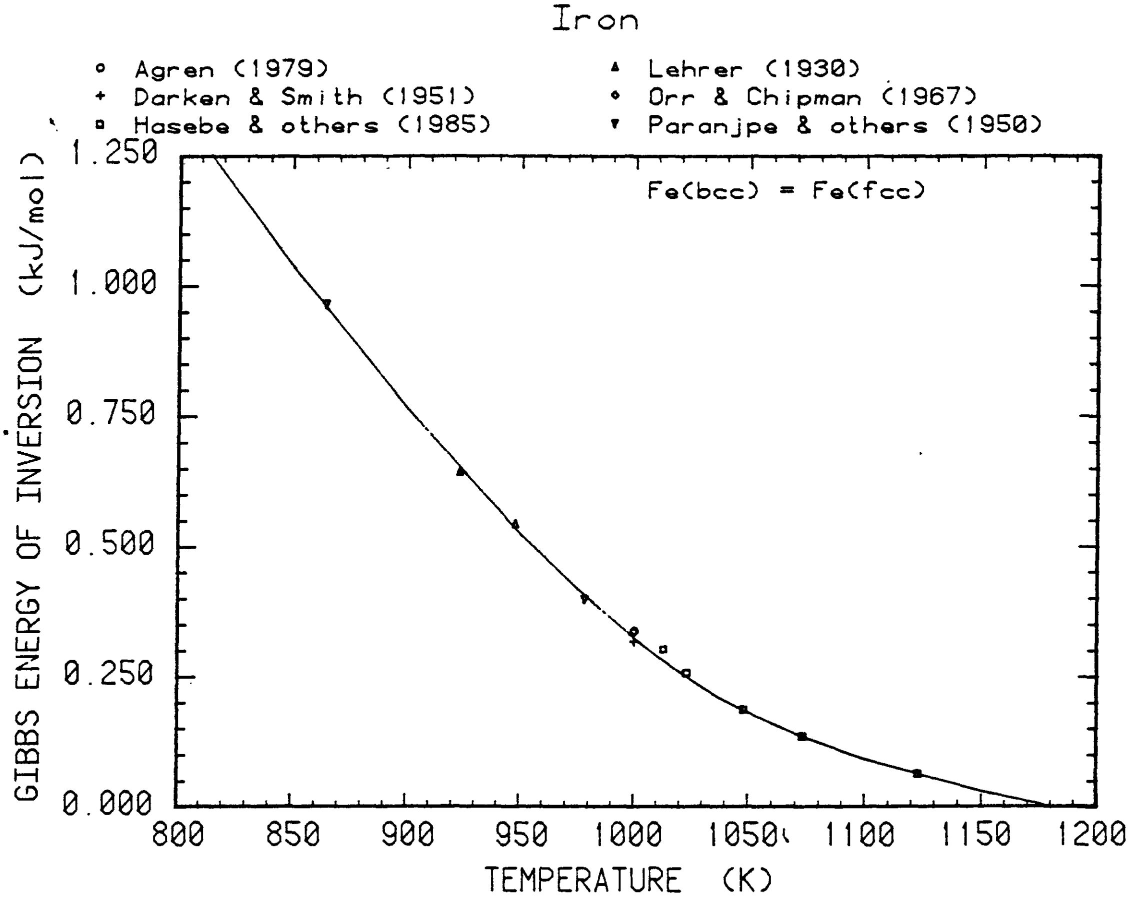


Figure 40. Comparison of the calculated difference between the Gibbs energy of Fe(bcc) and Fe(fcc) and reported data from analyses of alloy chemistry.

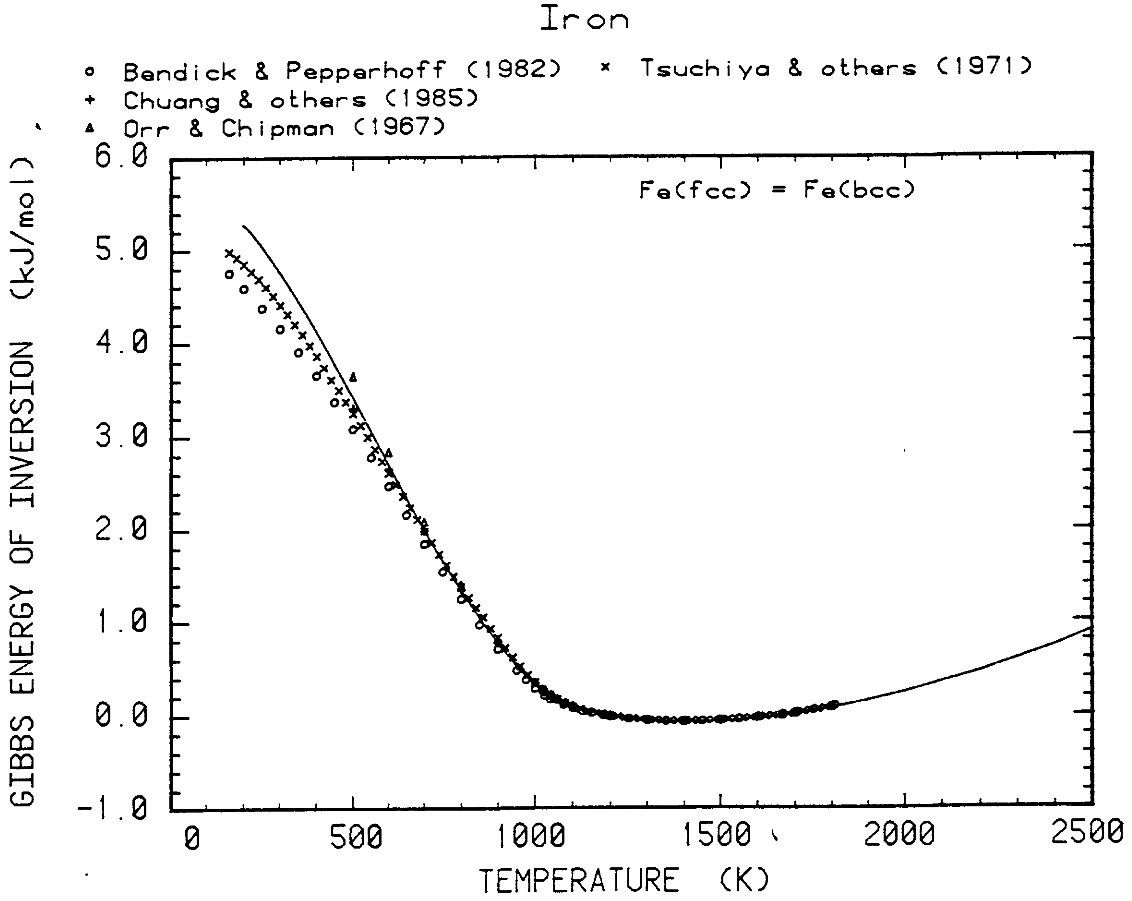


Figure 41. Comparison of the calculated difference between the Gibbs energy of Fe(bcc) and Fe(fcc) and data reported in the literature.

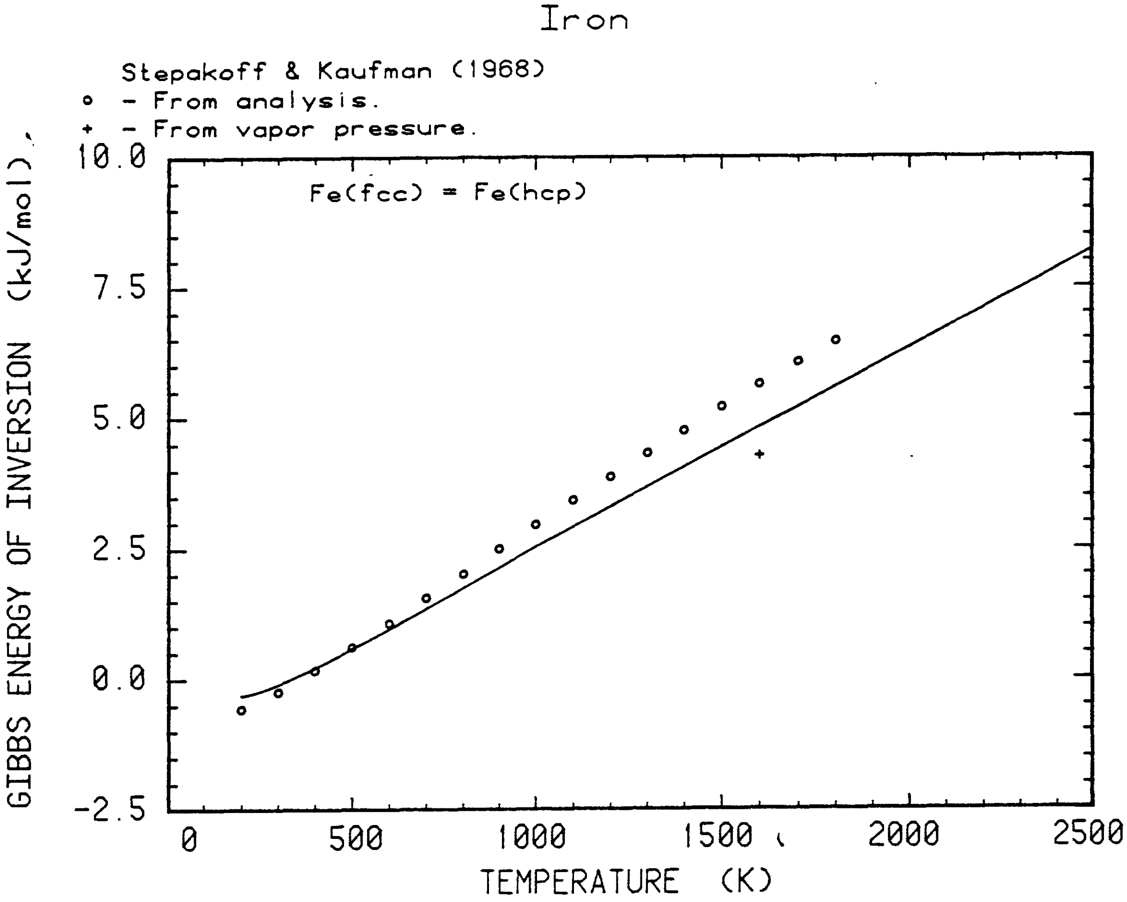


Figure 42. Comparison of the calculated difference between the Gibbs energy of Fe(bcc) and Fe(hcp) and data reported by Stepakoff and Kaufman (1968).

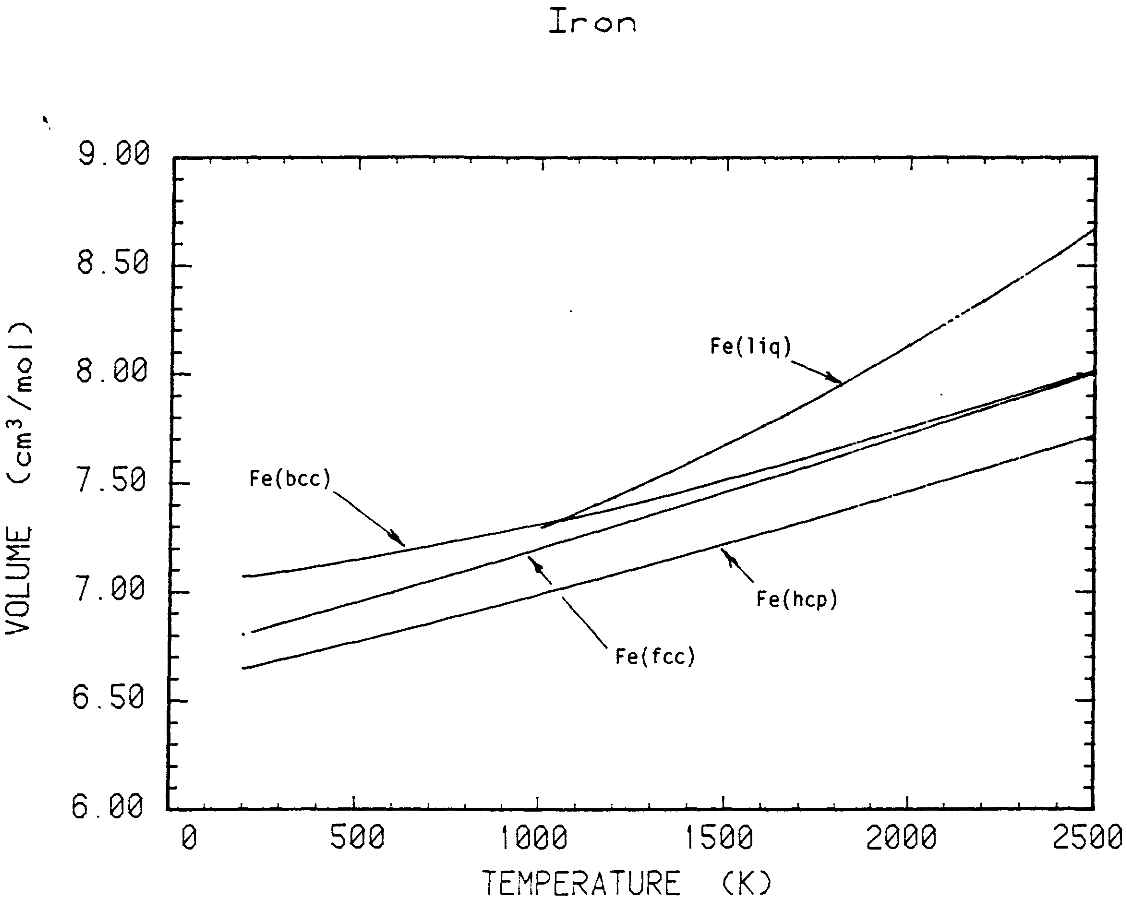


Figure 43. Plot of the calculated molar volumes of the three solids and of Fe(liq).

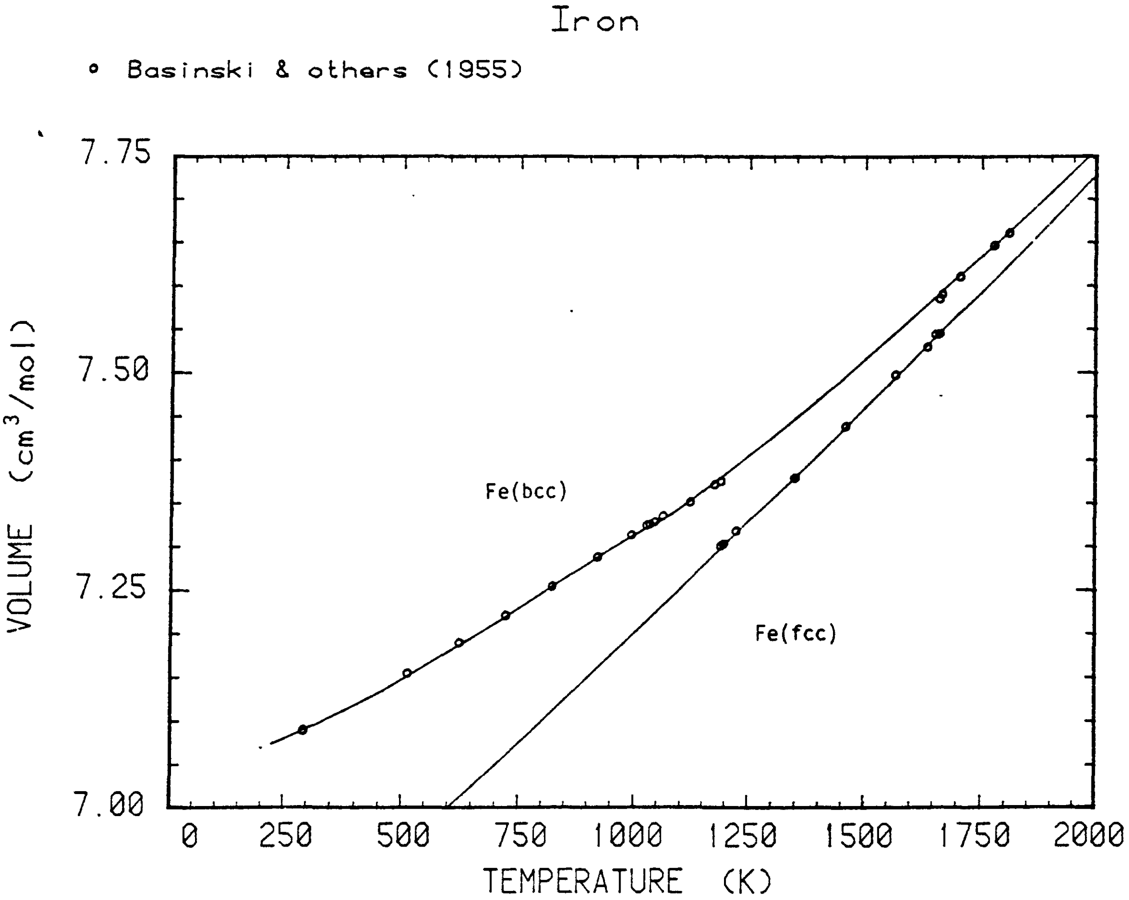


Figure 44. Comparison of the calculated molar volumes with the experimental data reported by Basinski and others (1955).

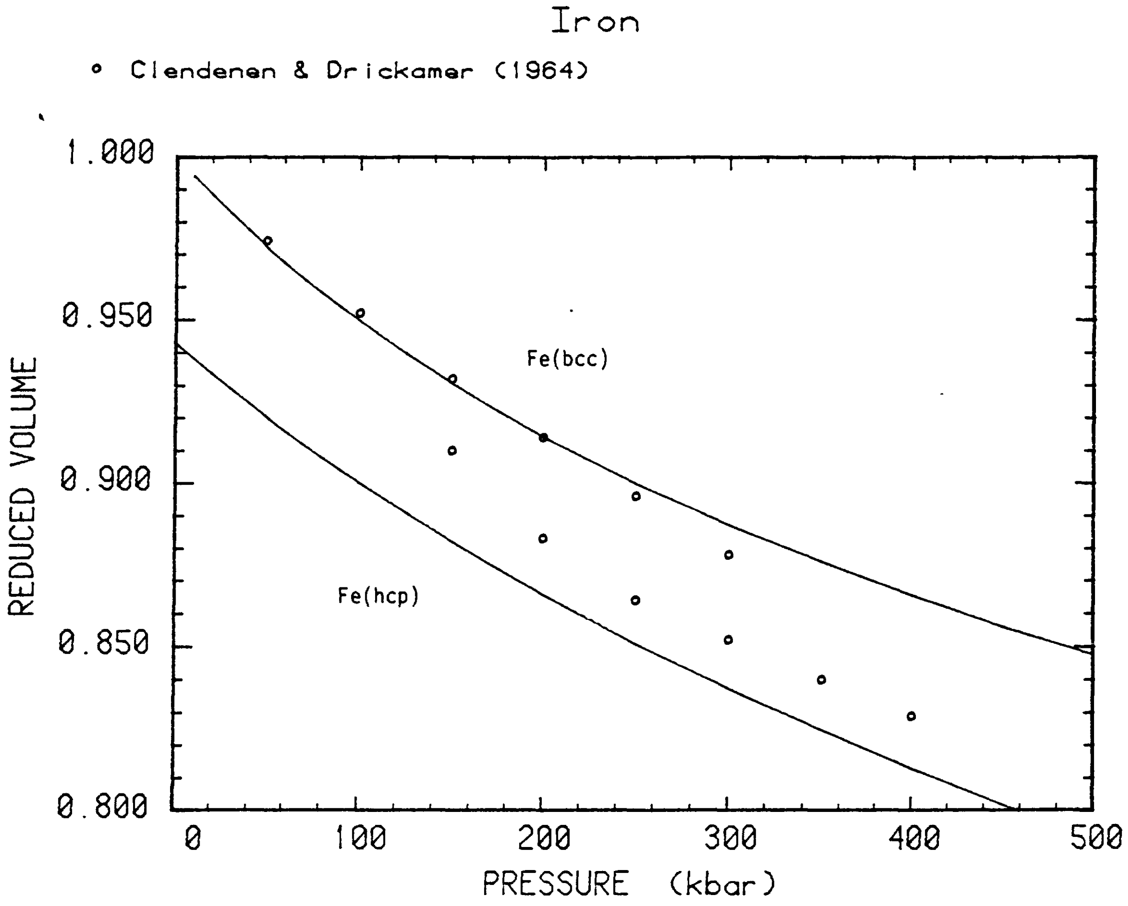


Figure 45. Comparison of the calculated molar volumes with the experimental data reported by Clendenen and Drickamer (1964).

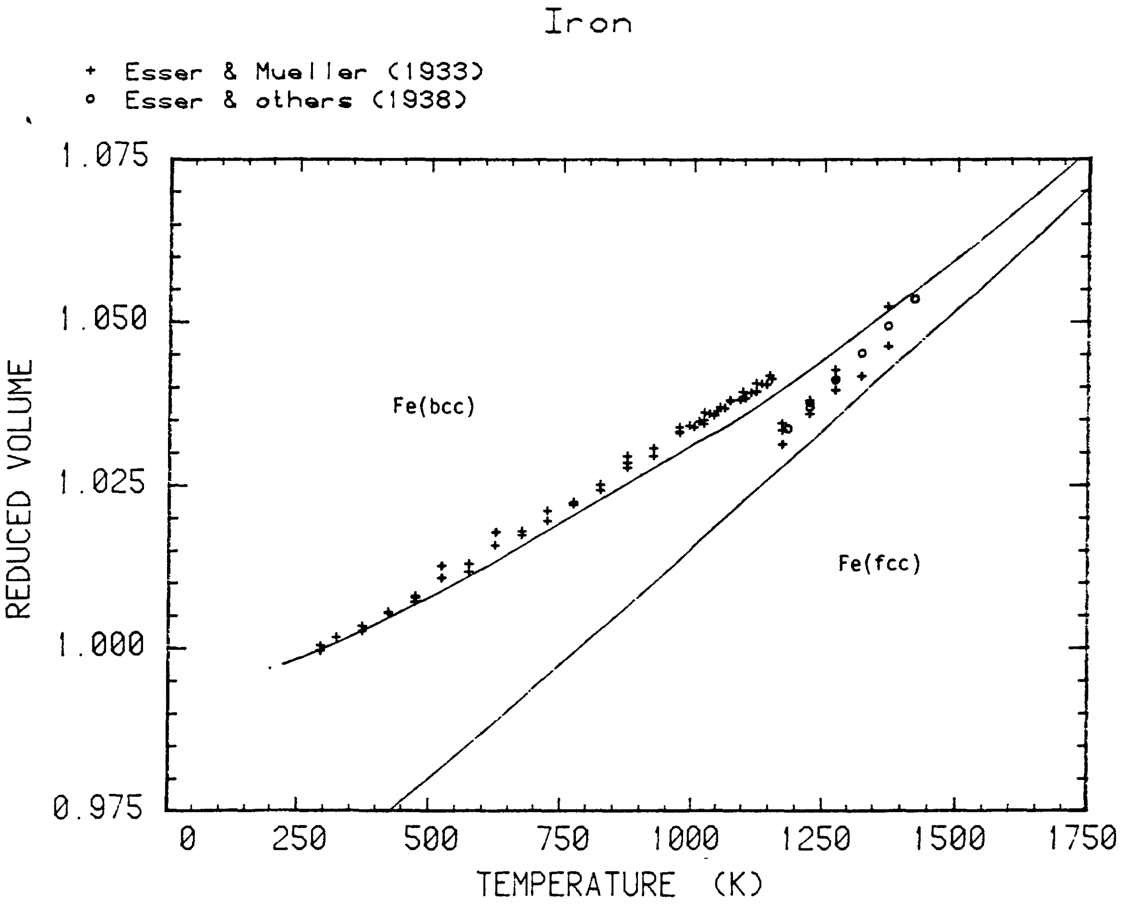


Figure 46. Comparison of the calculated molar volumes with the experimental data reported by Esser and Mueller (1933) and Esser and others (1938).

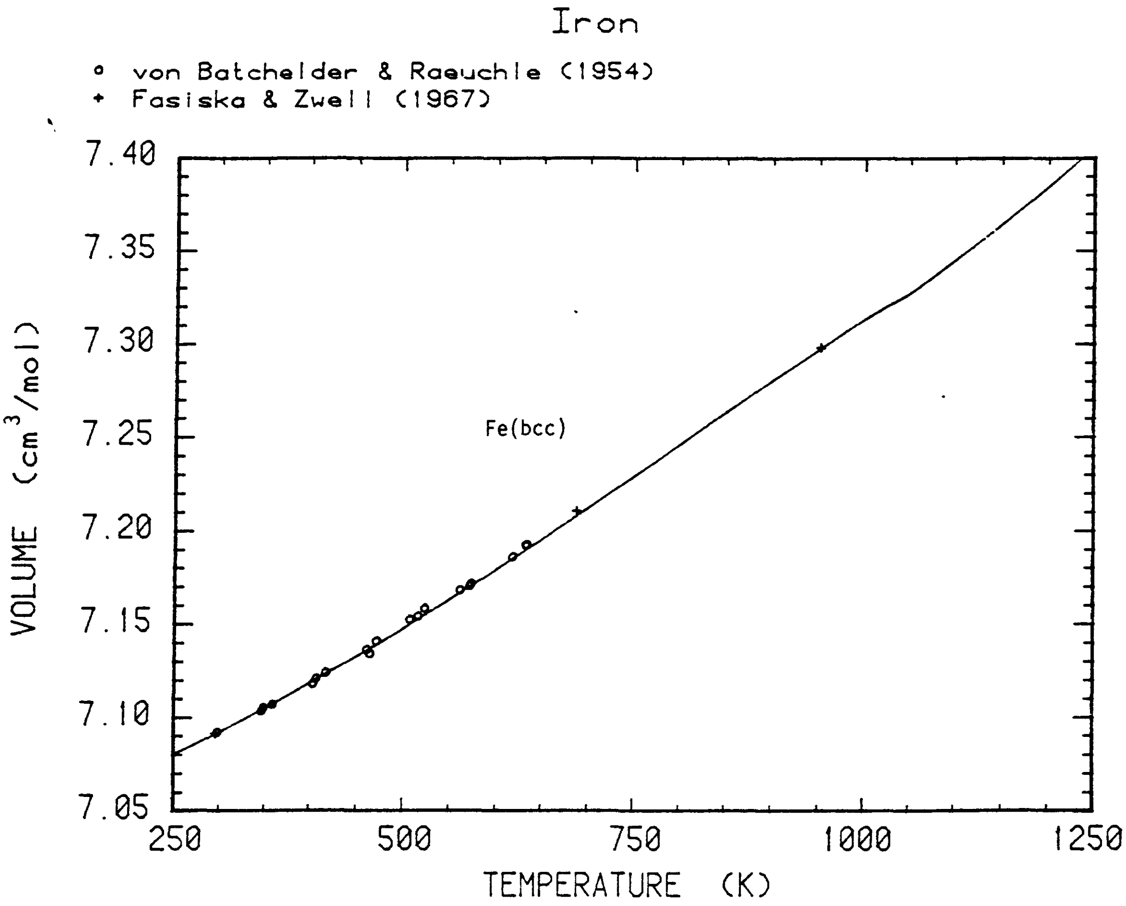


Figure 47. Comparison of the calculated molar volumes with the experimental data reported by Fasiska and Zwell (1967) and von Batchelder and Raeuchle (1954).

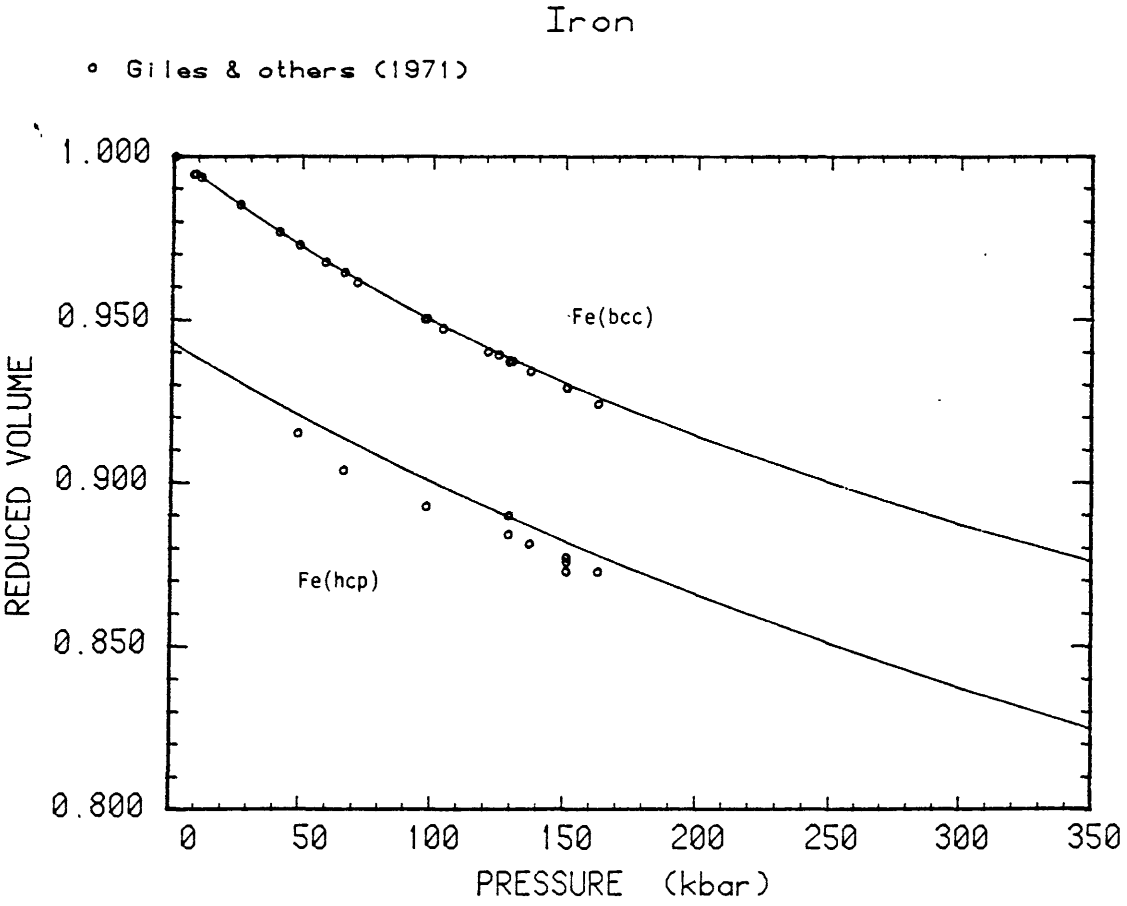


Figure 48. Comparison of the calculated molar volumes with the experimental data reported by Giles and others (1971).

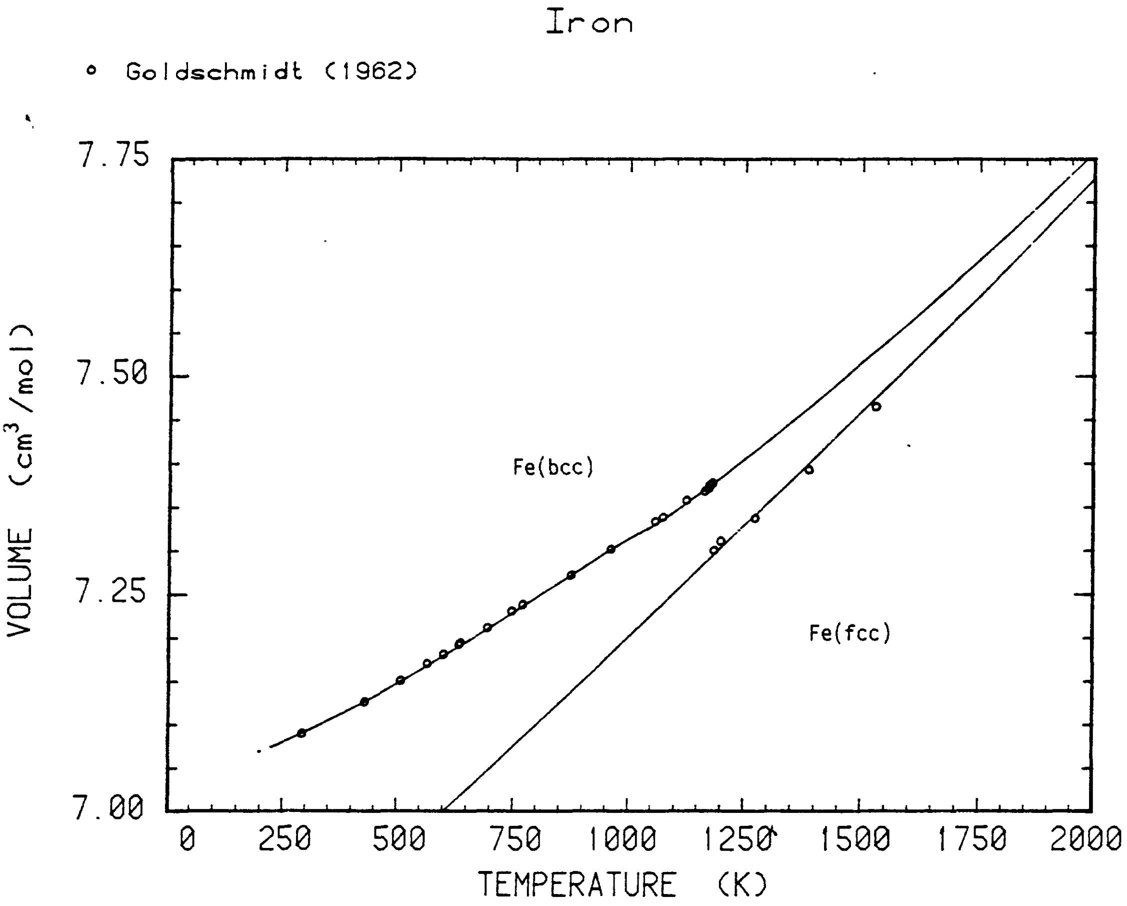


Figure 49. Comparison of the calculated molar volumes with the experimental data reported by Goldschmidt (1962).

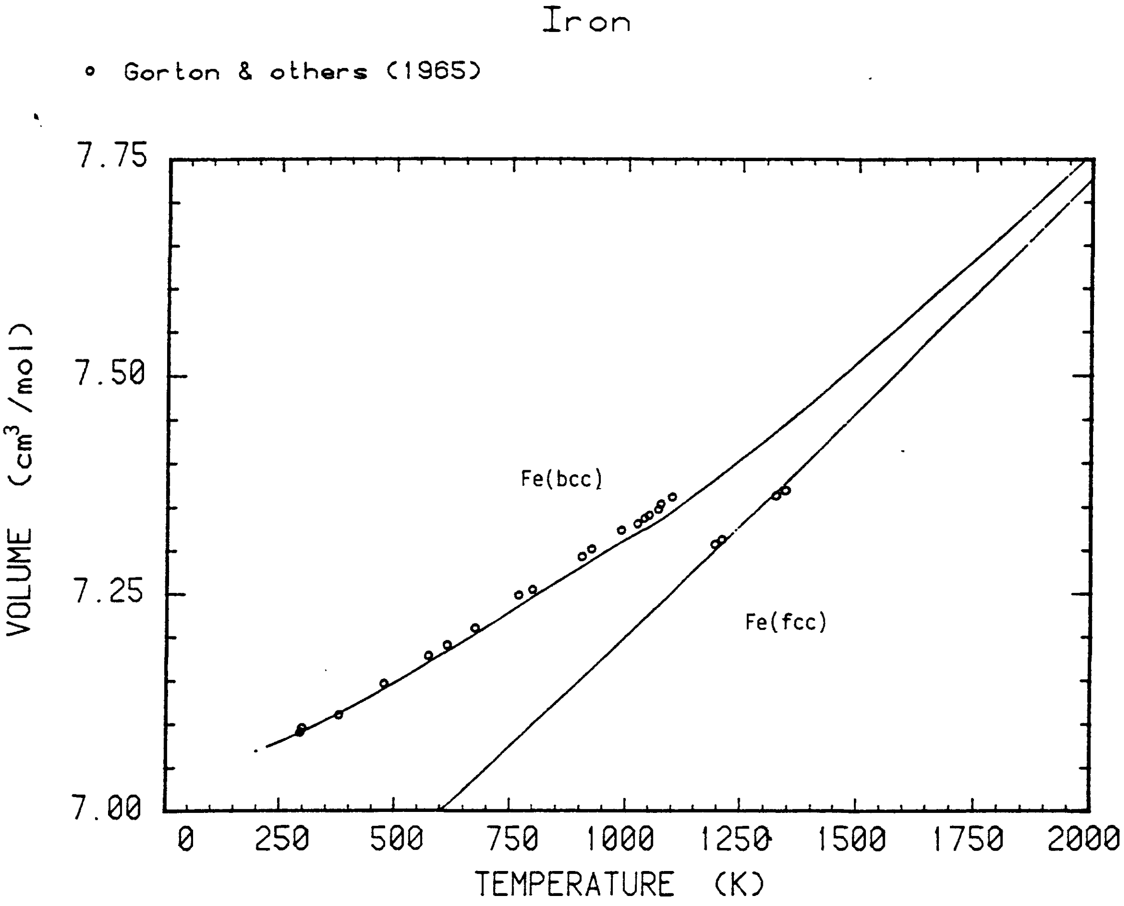


Figure 50. Comparison of the calculated molar volumes with the experimental data reported by Gorton and others (1965).

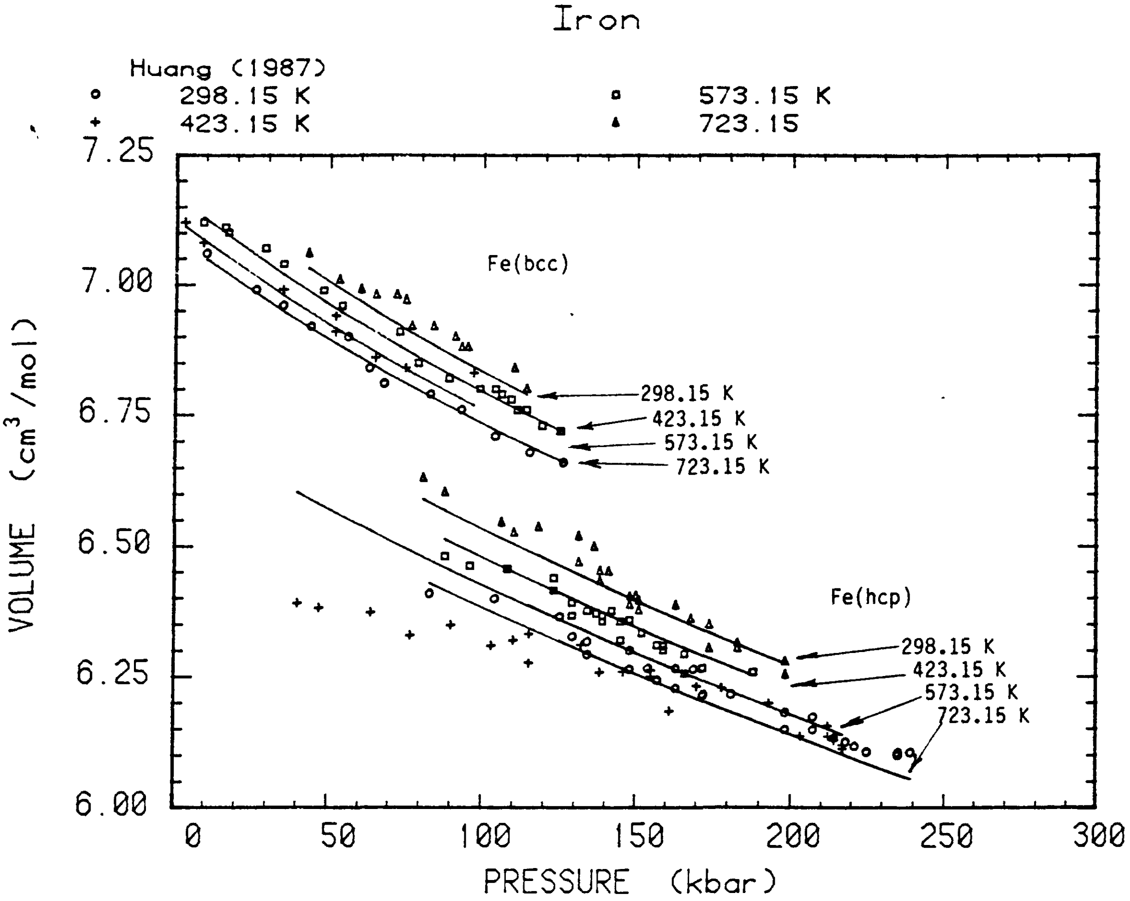


Figure 51. Comparison of the calculated molar volumes with the experimental data reported by Huang (1987) and Huang and others (1987).

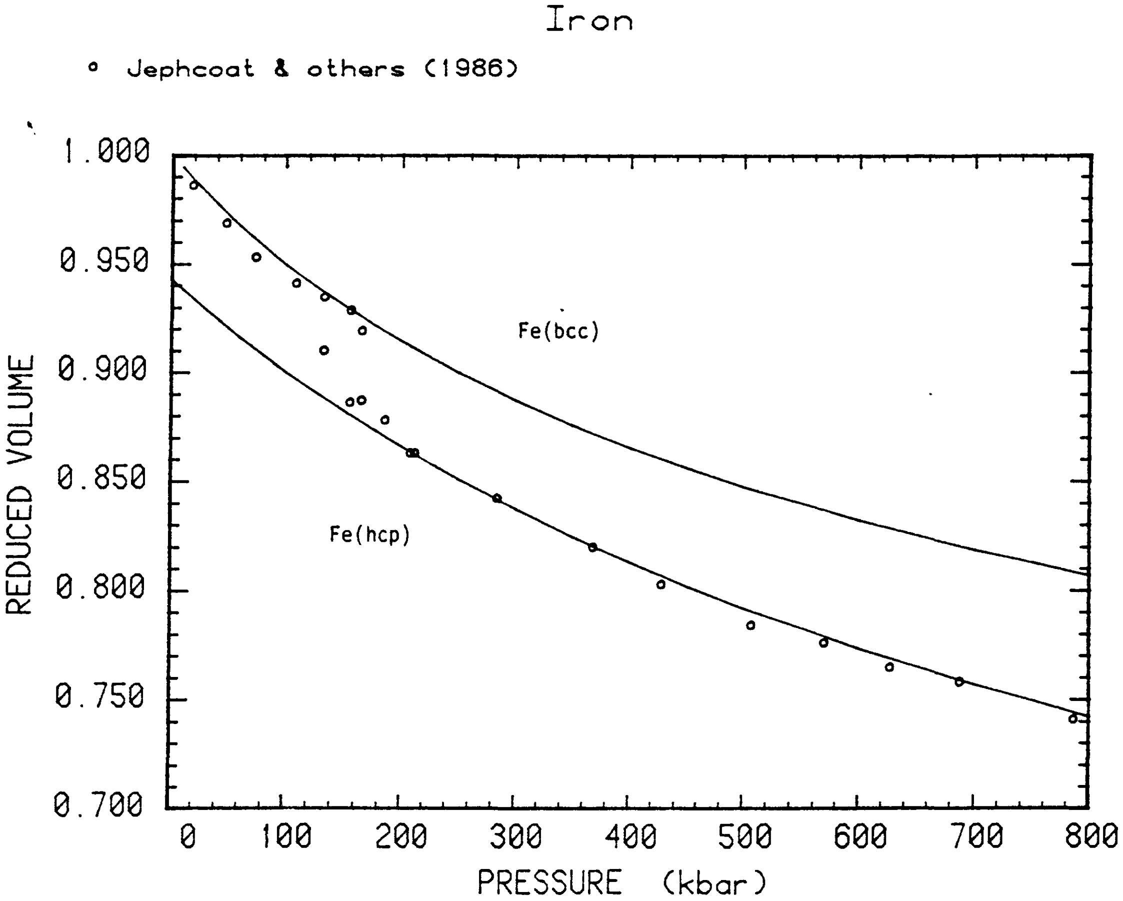


Figure 52. Comparison of the calculated molar volumes with the experimental data reported by Jephcoat and others (1986).

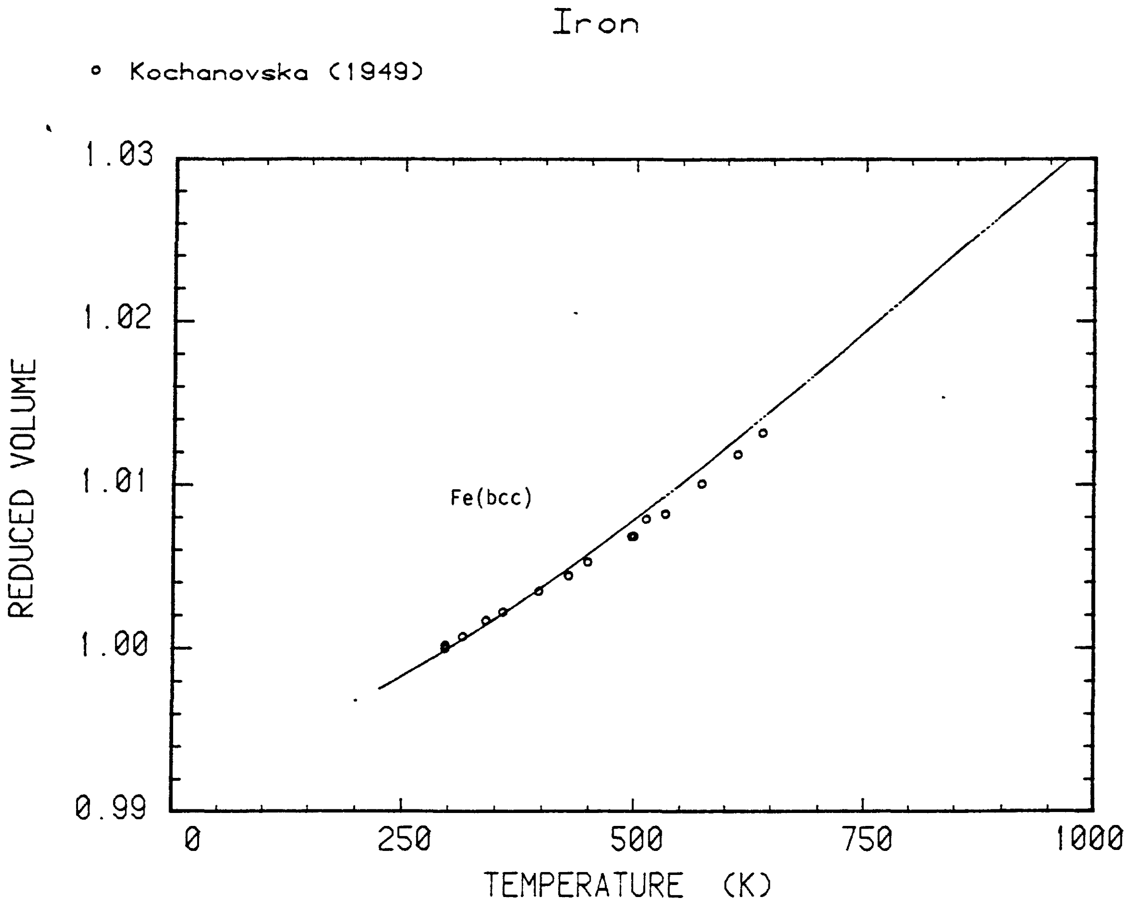


Figure 53. Comparison of the calculated molar volumes with the experimental data reported by Kochanovskå (1949).

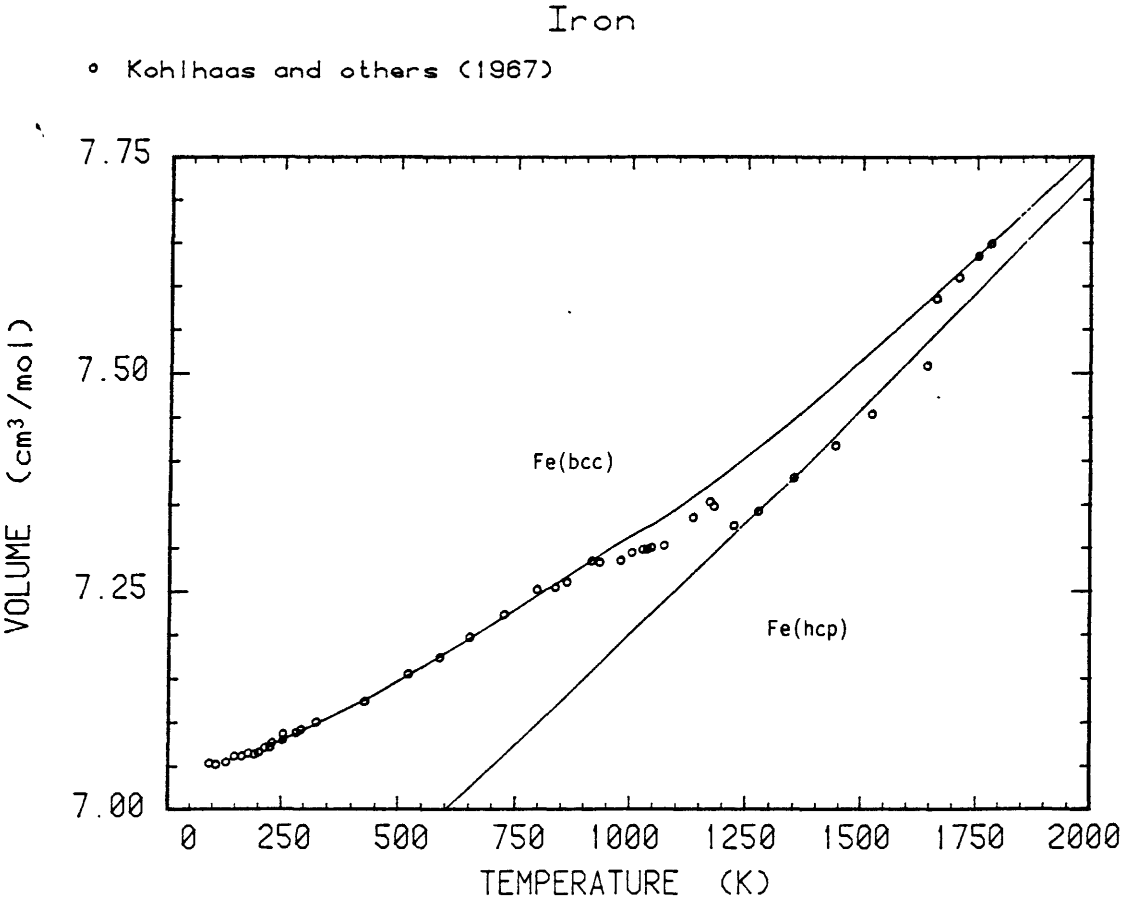


Figure 54. Comparison of the calculated molar volumes with the experimental data reported by Kohlhaas and others (1967).

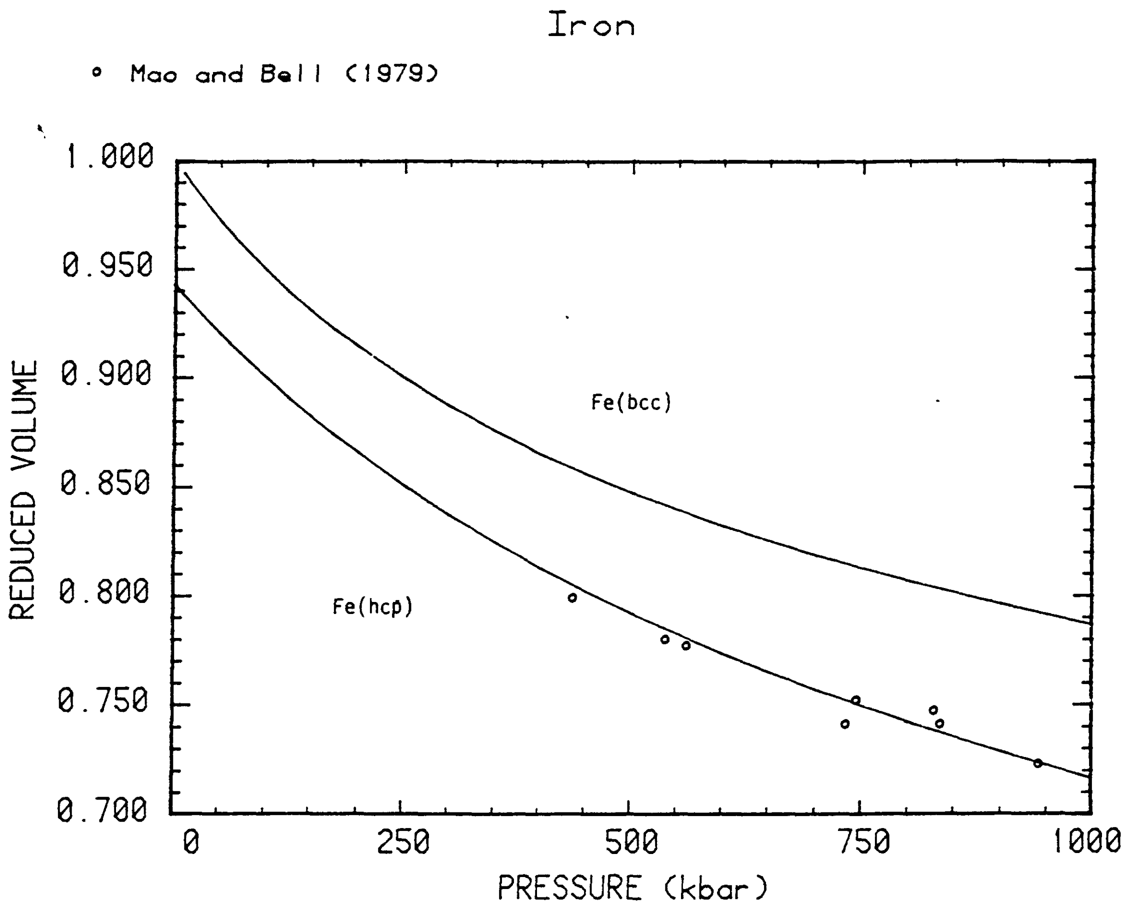


Figure 55. Comparison of the calculated molar volumes with the experimental data reported by Mao and Bell (1979).

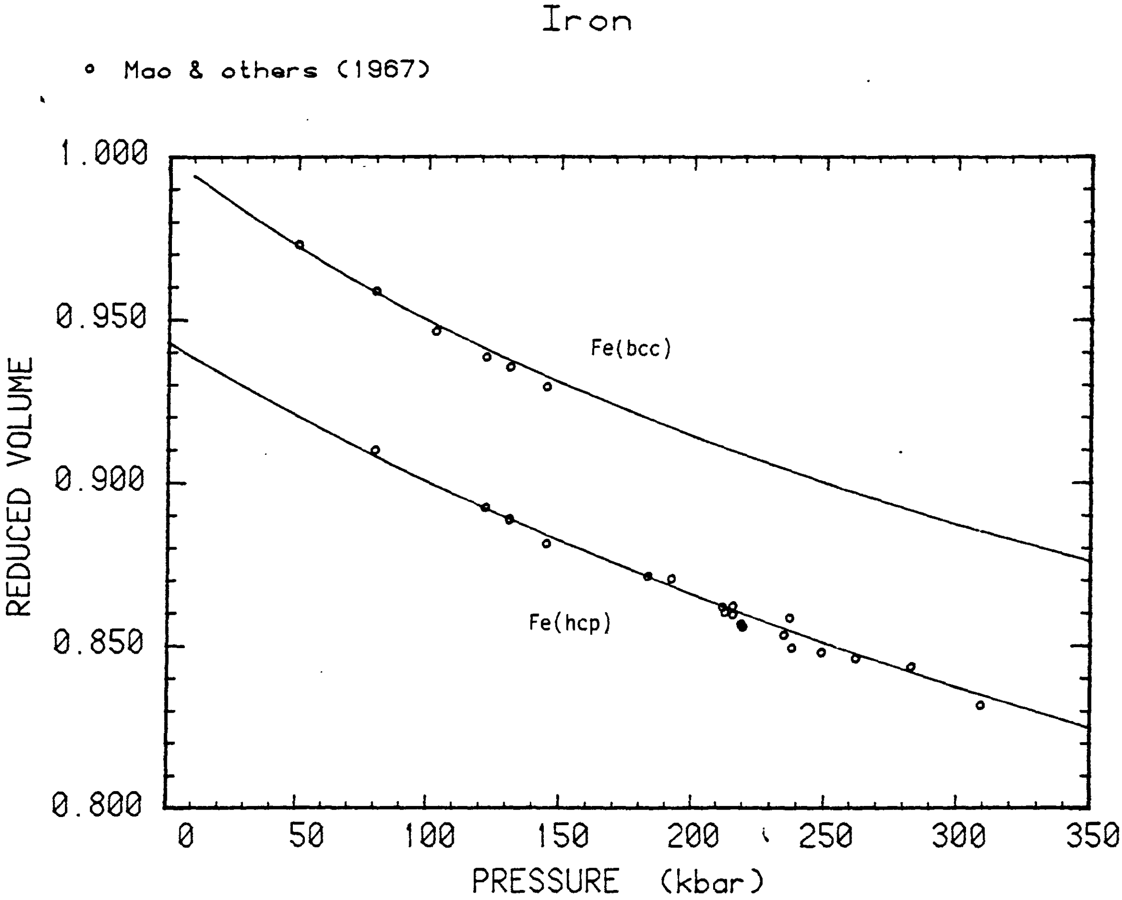


Figure 56. Comparison of the calculated molar volumes with the experimental data reported by Mao and others (1967).

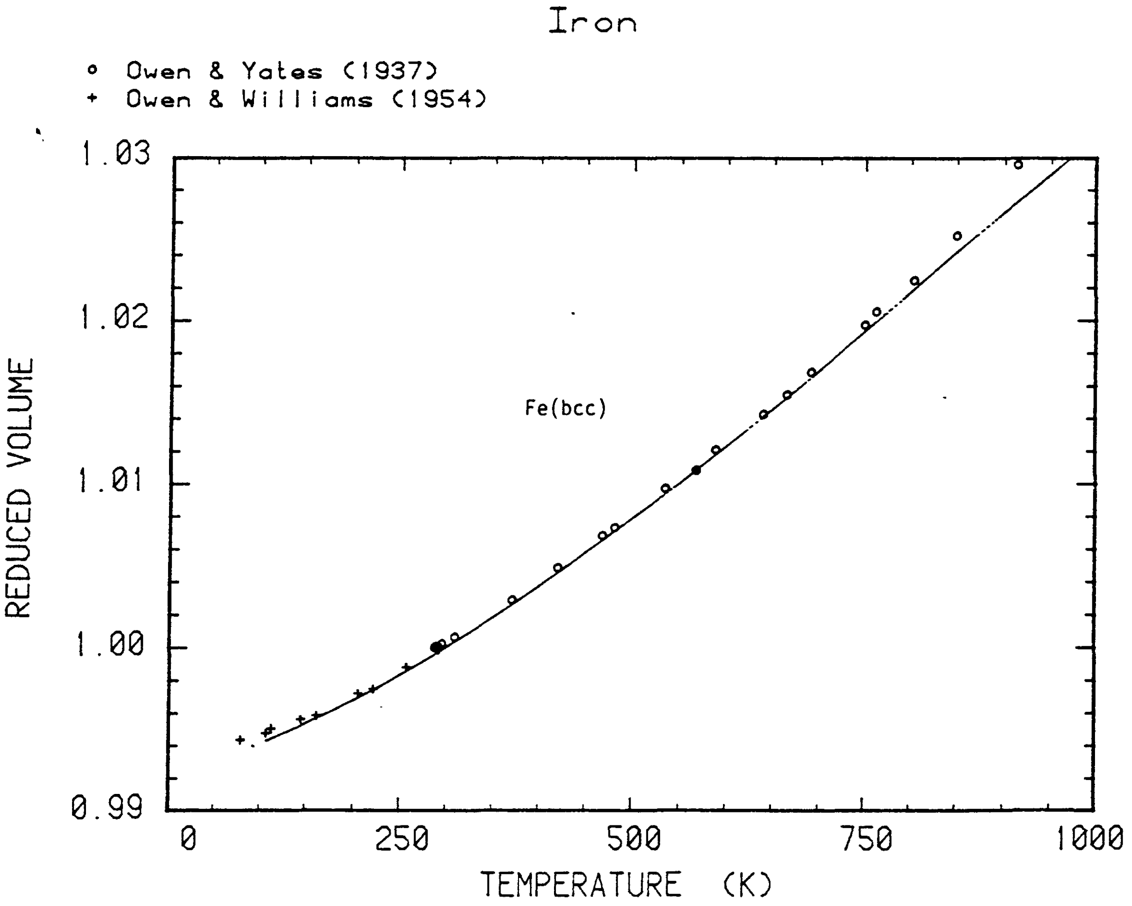


Figure 57. Comparison of the calculated molar volumes with the experimental data reported by Owen and Williams (1954) and Owen and Yates (1937).

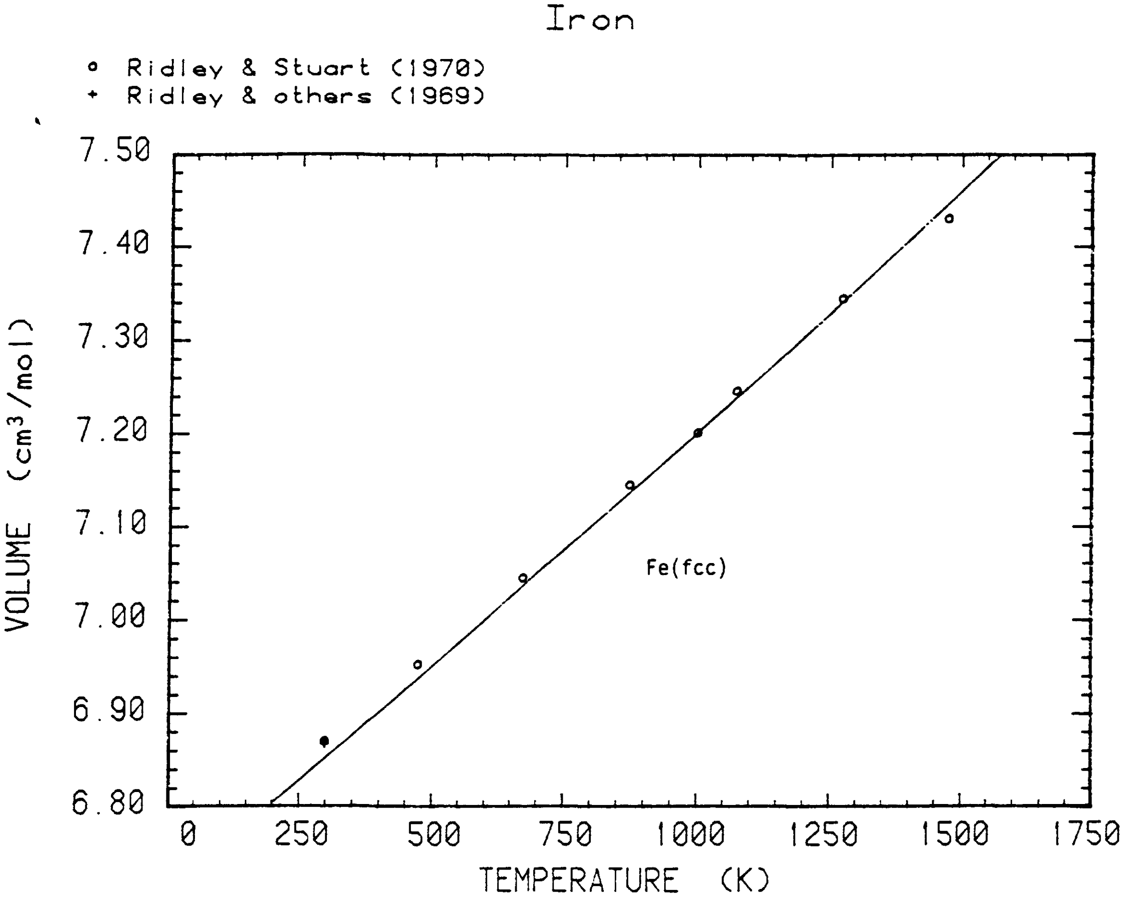


Figure 58. Comparison of the calculated molar volumes with the experimental data reported by Ridley and others (1969) and Ridley and Stuart (1970).

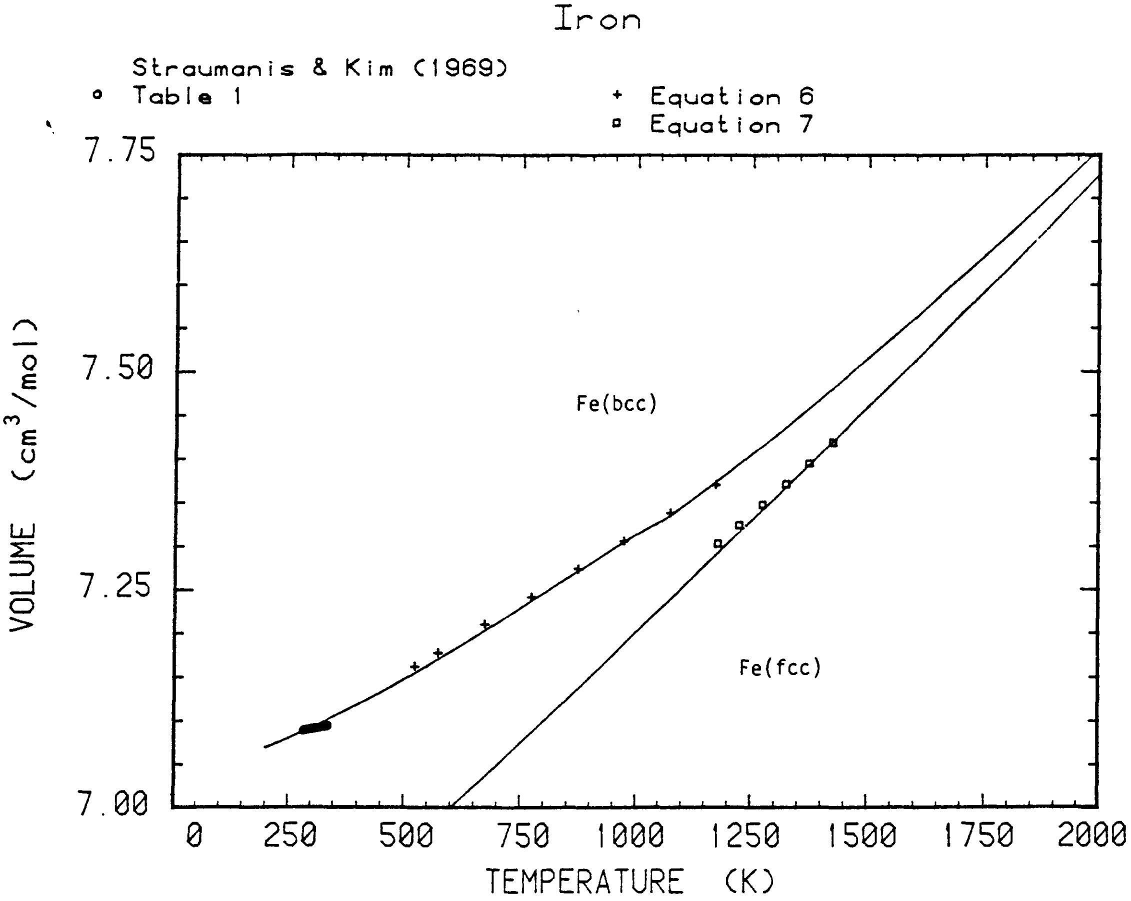


Figure 59. Comparison of the calculated molar volumes with the experimental data reported by Straumanis and Kim (1969).

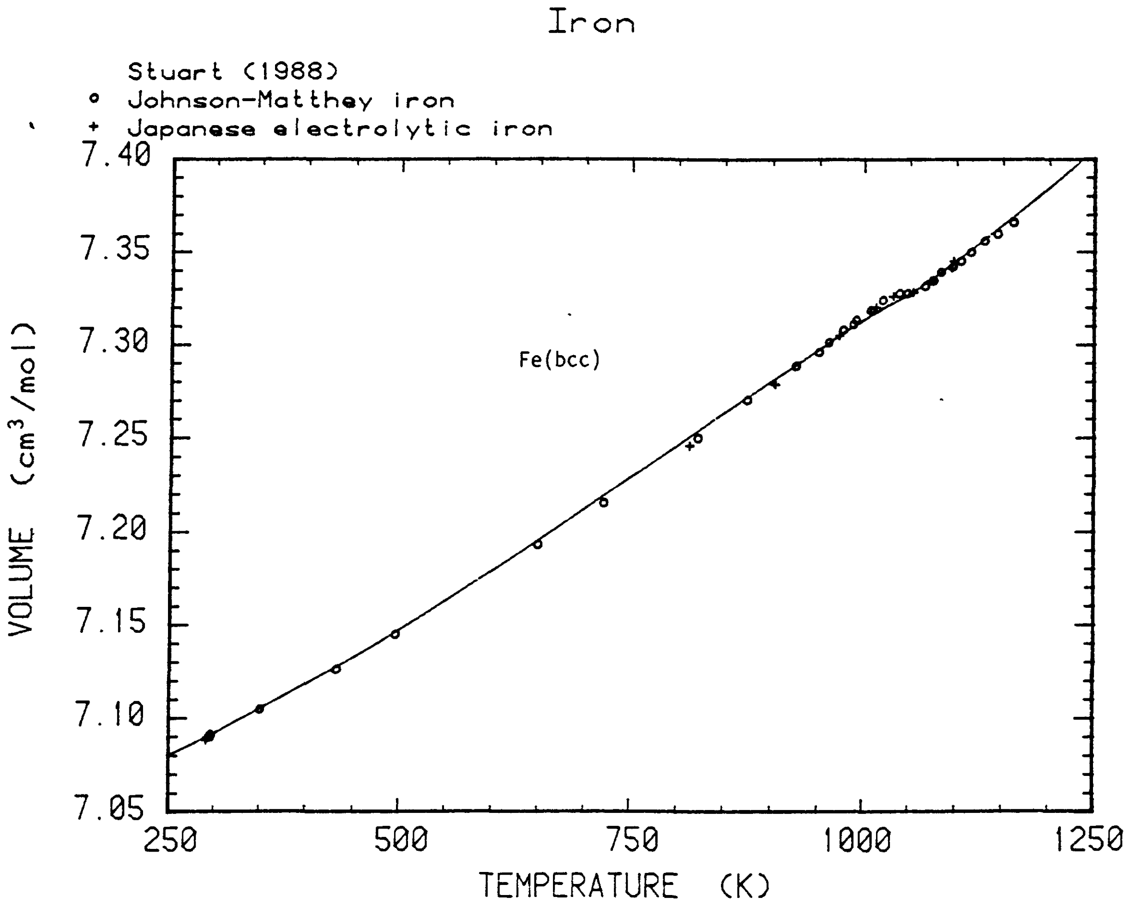


Figure 60. Comparison of the calculated molar volumes with the experimental data reported by Stuart (1988).

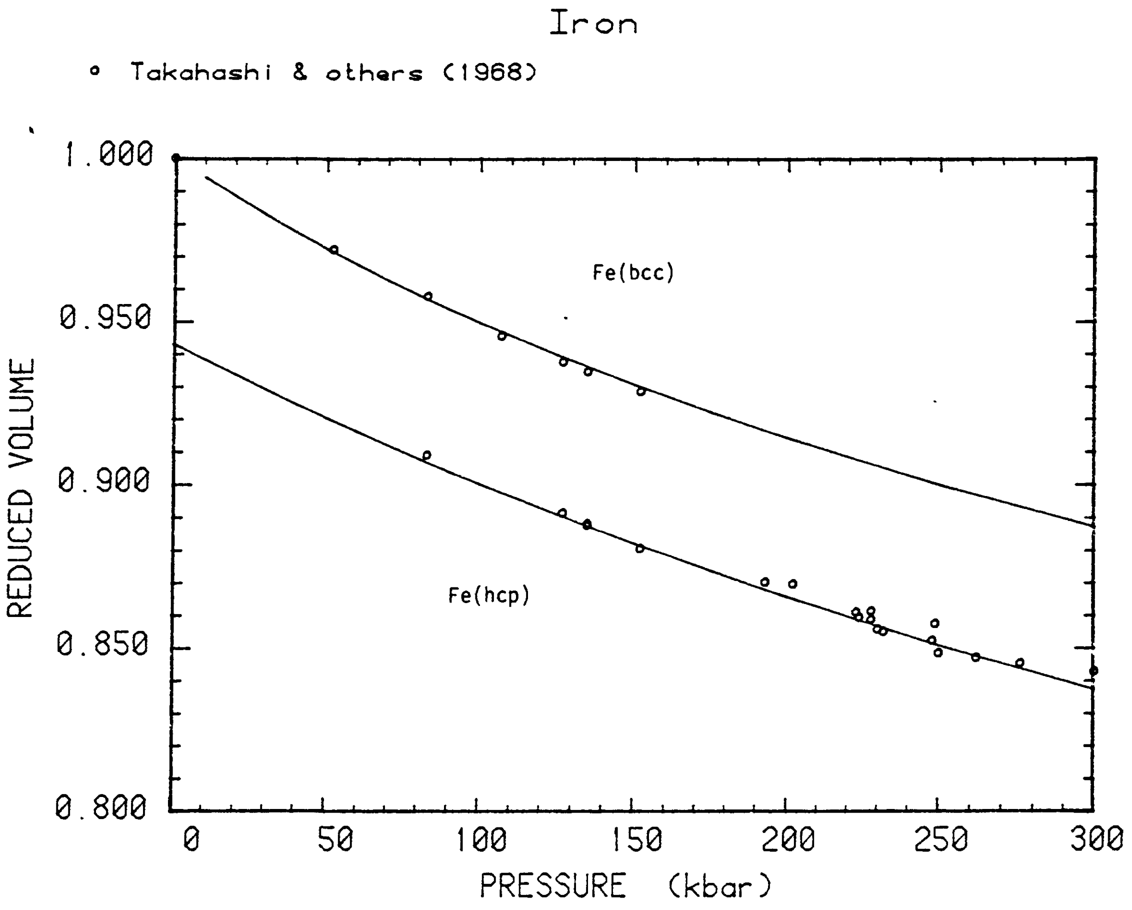


Figure 61. Comparison of the calculated molar volumes with the experimental data reported by Takahashi and others (1968).

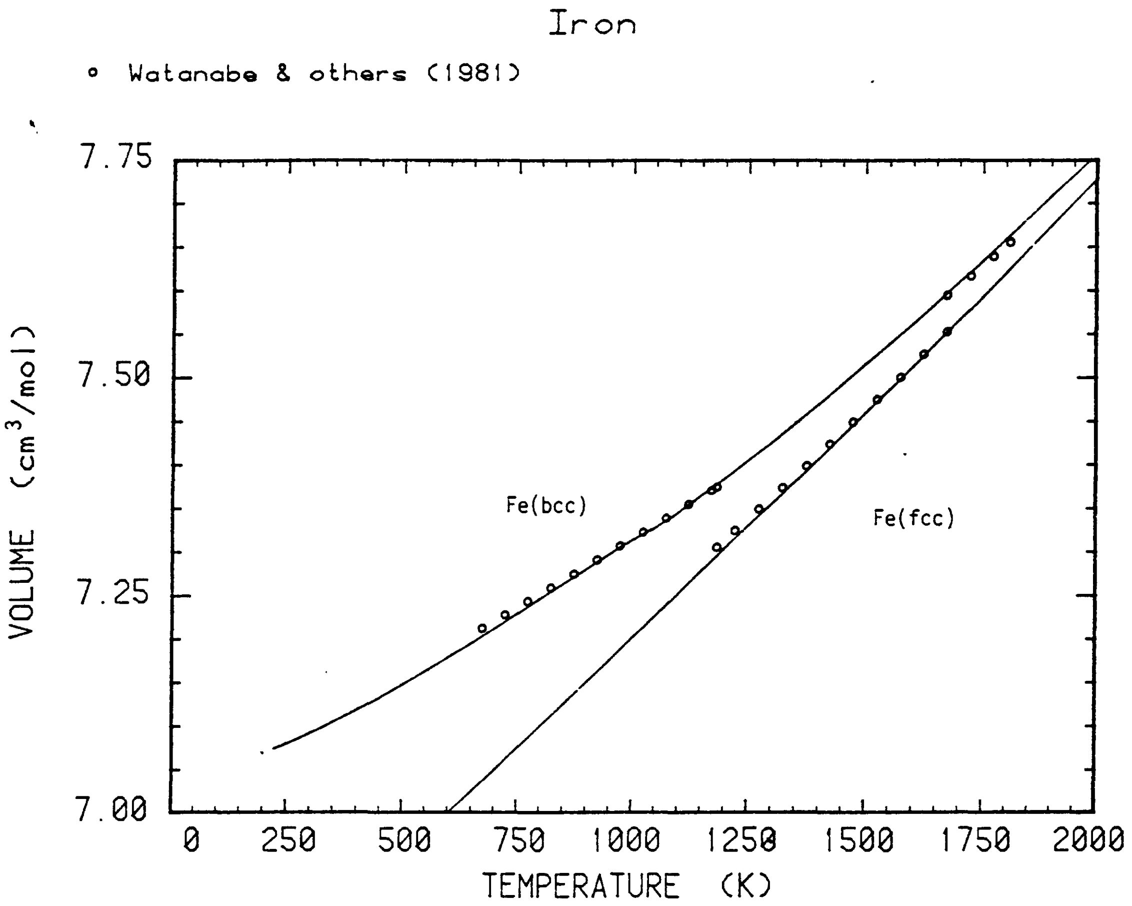


Figure 62. Comparison of the calculated molar volumes with the experimental data reported by Watanabe and others (1981).

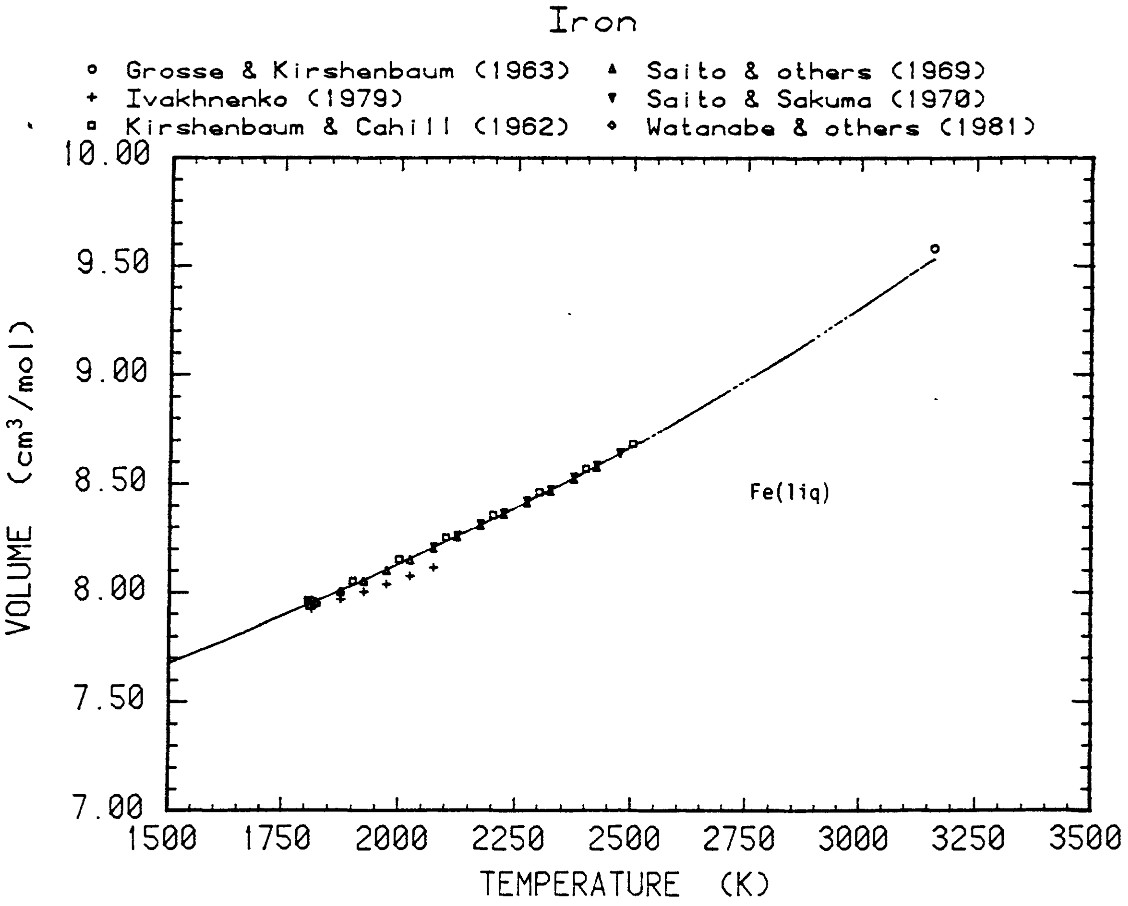


Figure 63. Comparison of the calculated molar volumes with the experimental data reported by Grosse and Kirshenbaum (1963), Ivakhnenko (1979), Kirshenbaum and Cahill (1962), Saito and others (1969), Saito and others (1970), and Watanabe and others (1981).

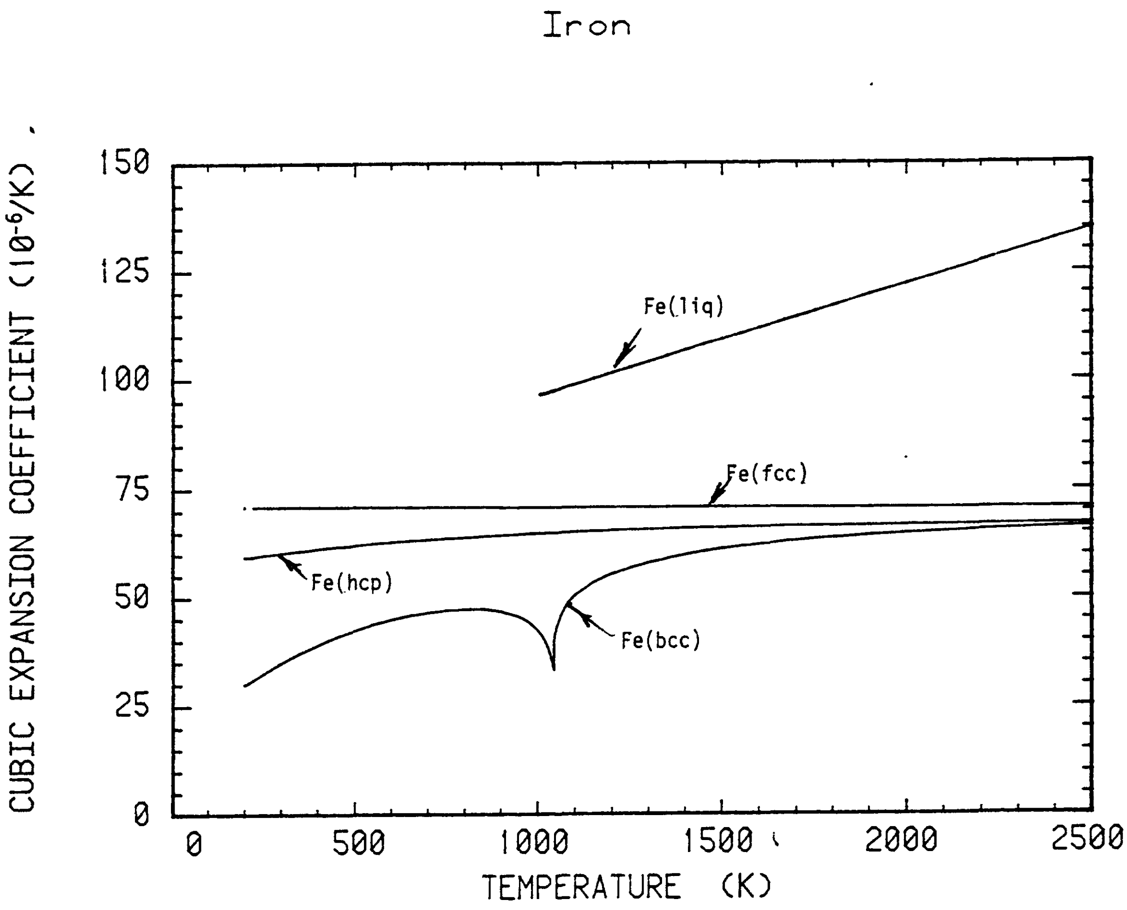


Figure 64. Plot of the calculated cubic expansion coefficient for the three solids and for Fe(liq).

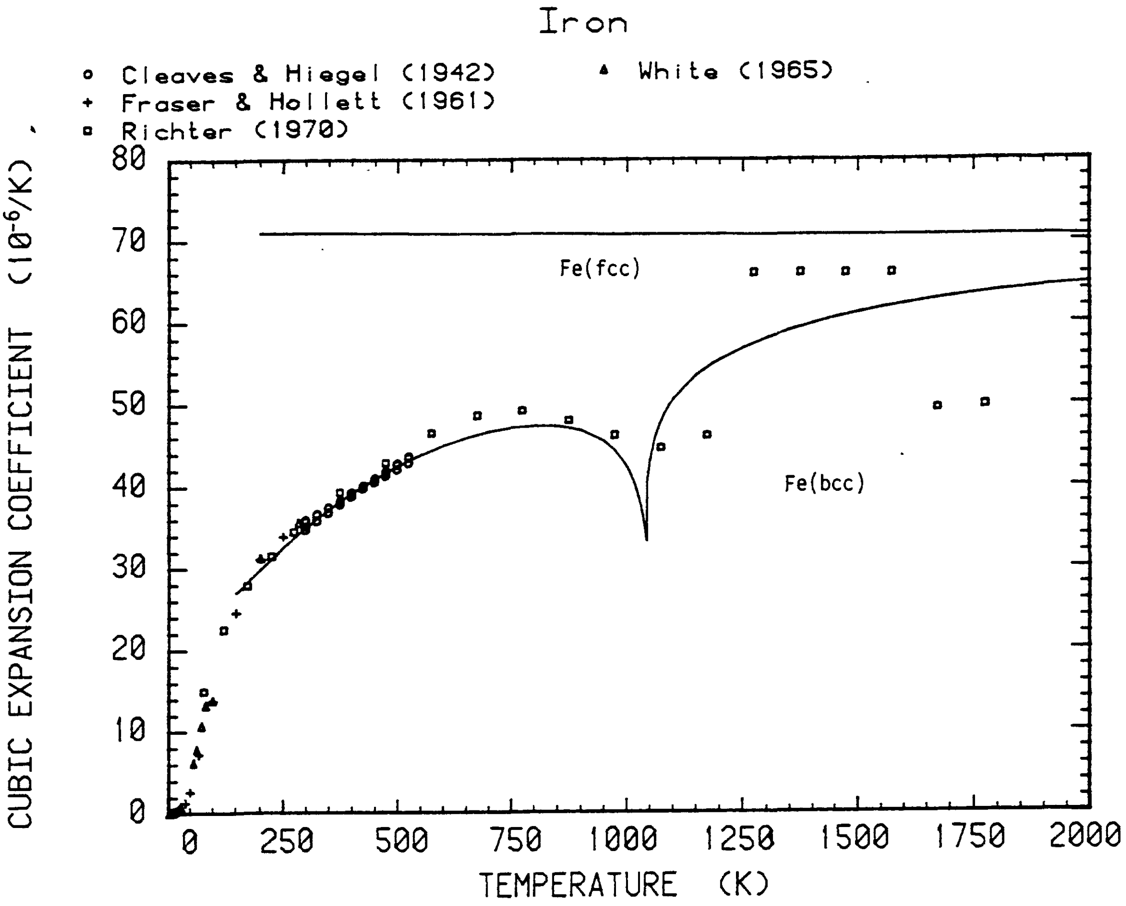


Figure 65. Comparison of the calculated cubic expansion coefficeint for Fe(bcc) and Fe(fcc) with the experimental data by Cleaves and Hiegel (1942), Fraser and Hollett (1961), Richter (1970), and White (1965).

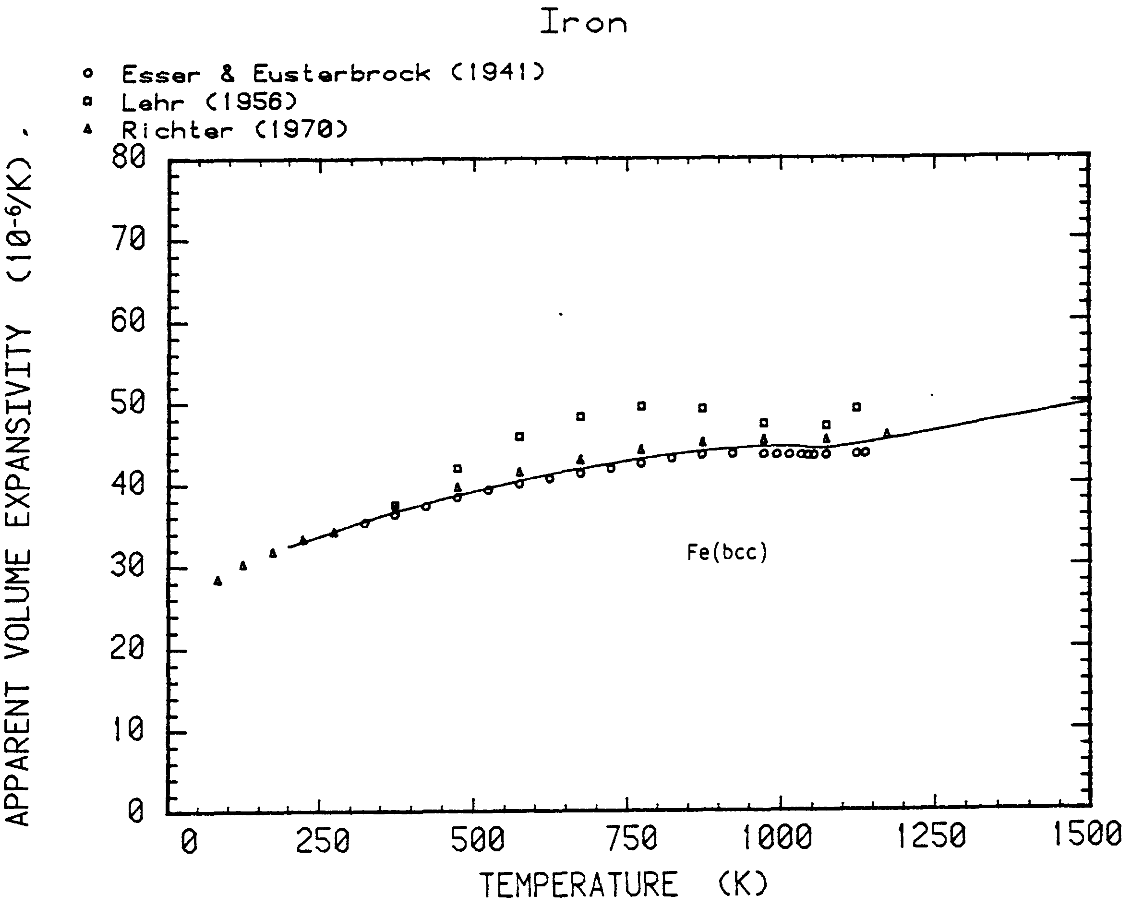


Figure 66. Comparison of the apparent volume expansivity with the experimental data by Esser and Eusterbrock (1941), Lehr (1956), and Richter (1970).

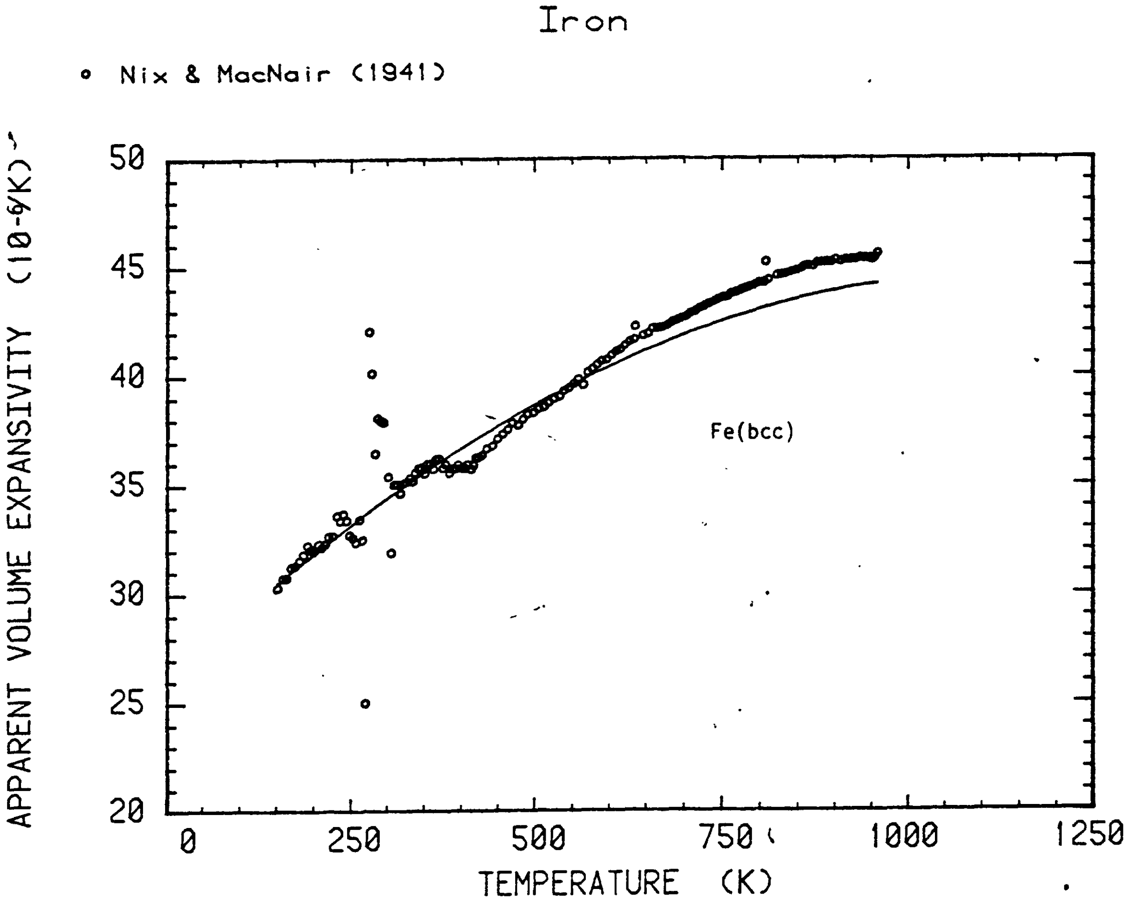


Figure 67. Comparison of the calculated apparent volume expansivity with the experimental data by Nix and MacNair (1941).

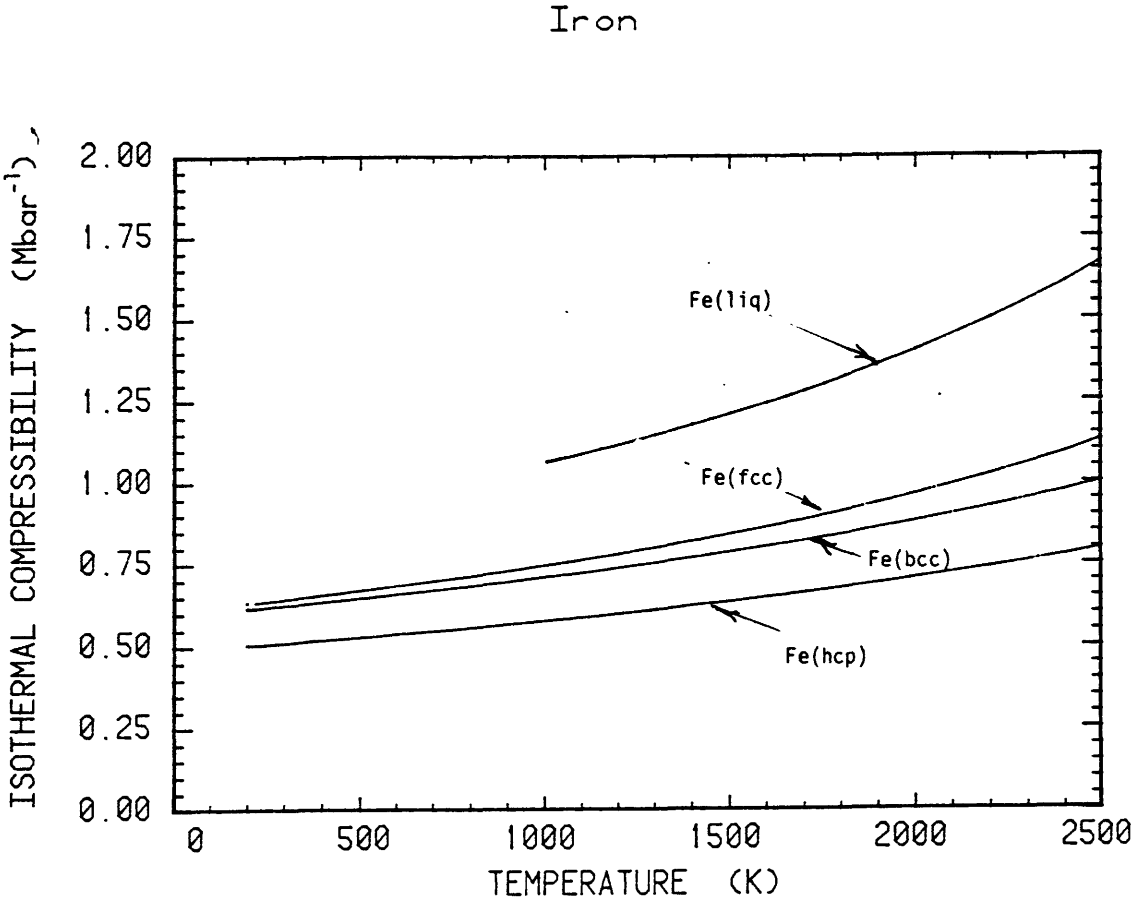


Figure 68. Calculated isothermal compressibility of the three solids and of Fe(liq).

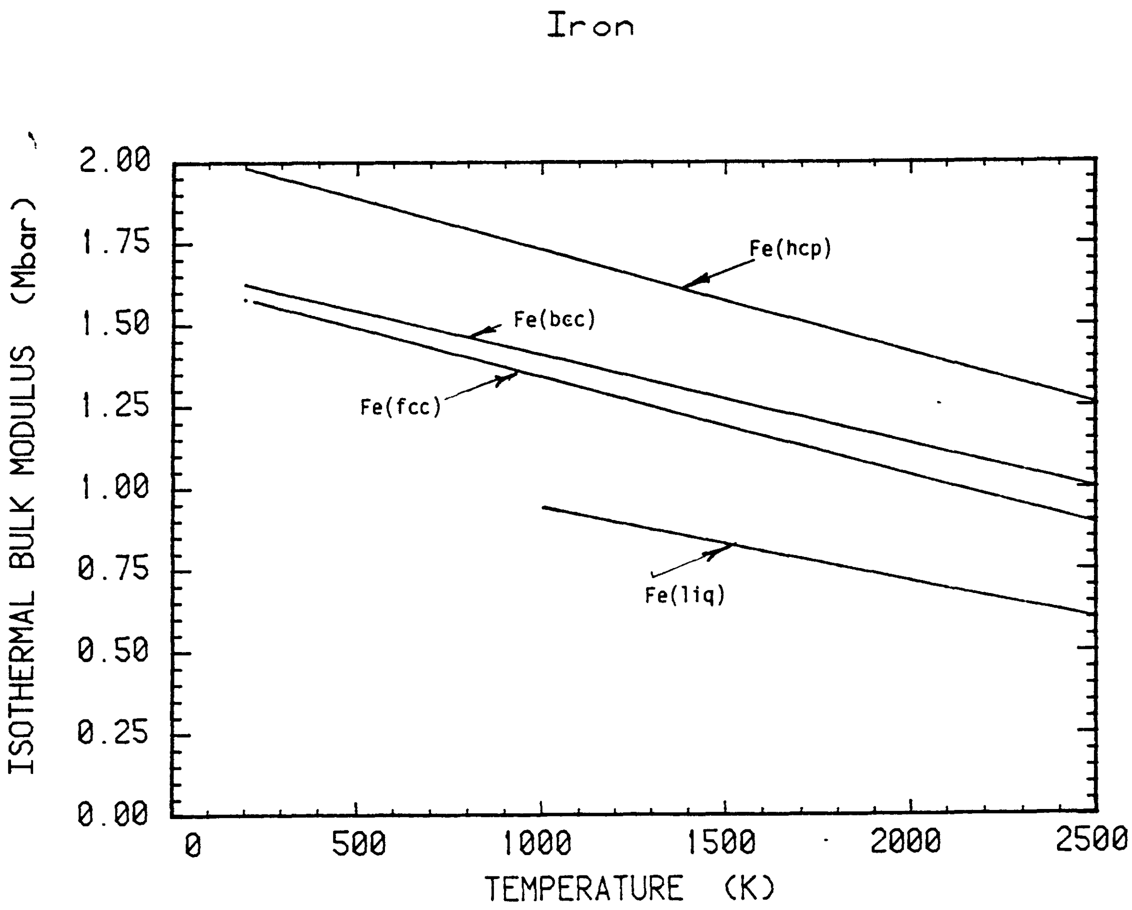


Figure 69. Plot of the calculated isotherman bulk modulus for the three solids and for Fe(liq).

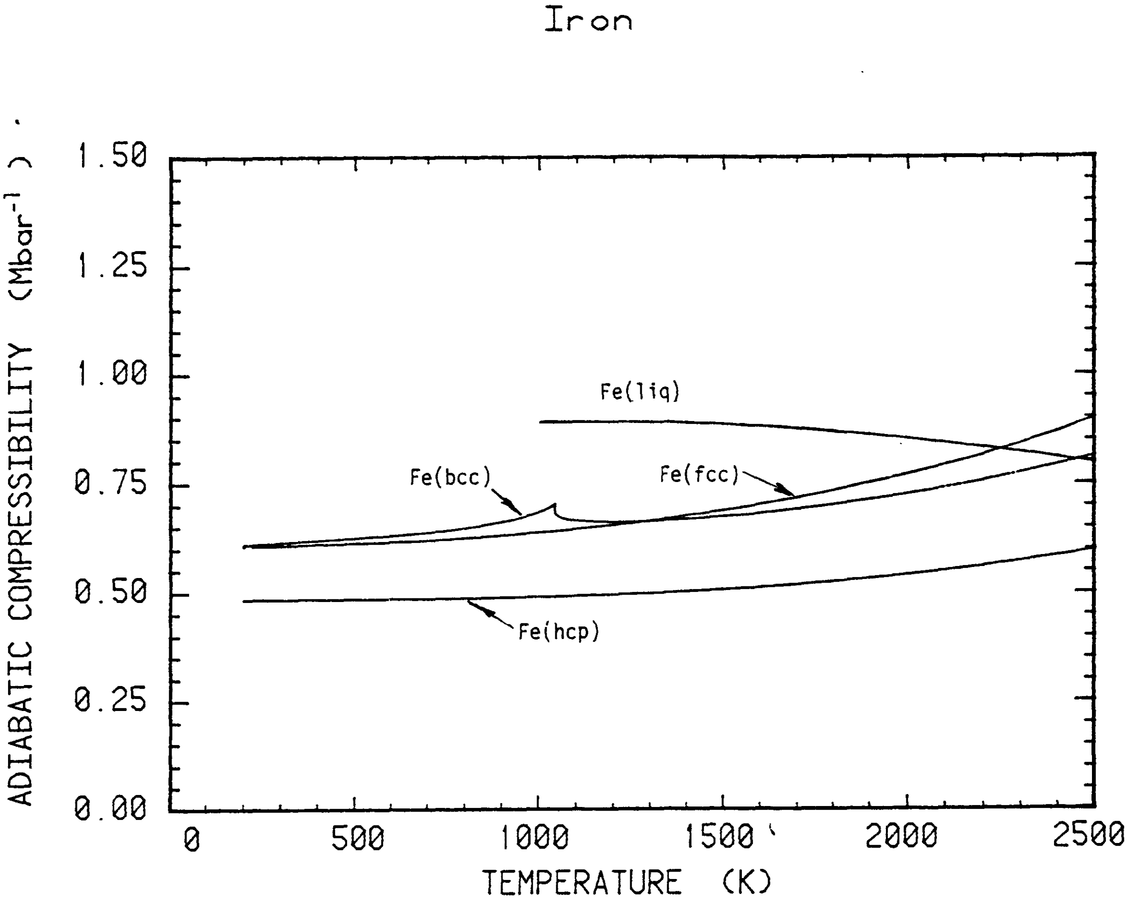


Figure 70. Plot of the isentropic compressiblity of the three solids and of Fe(liq).

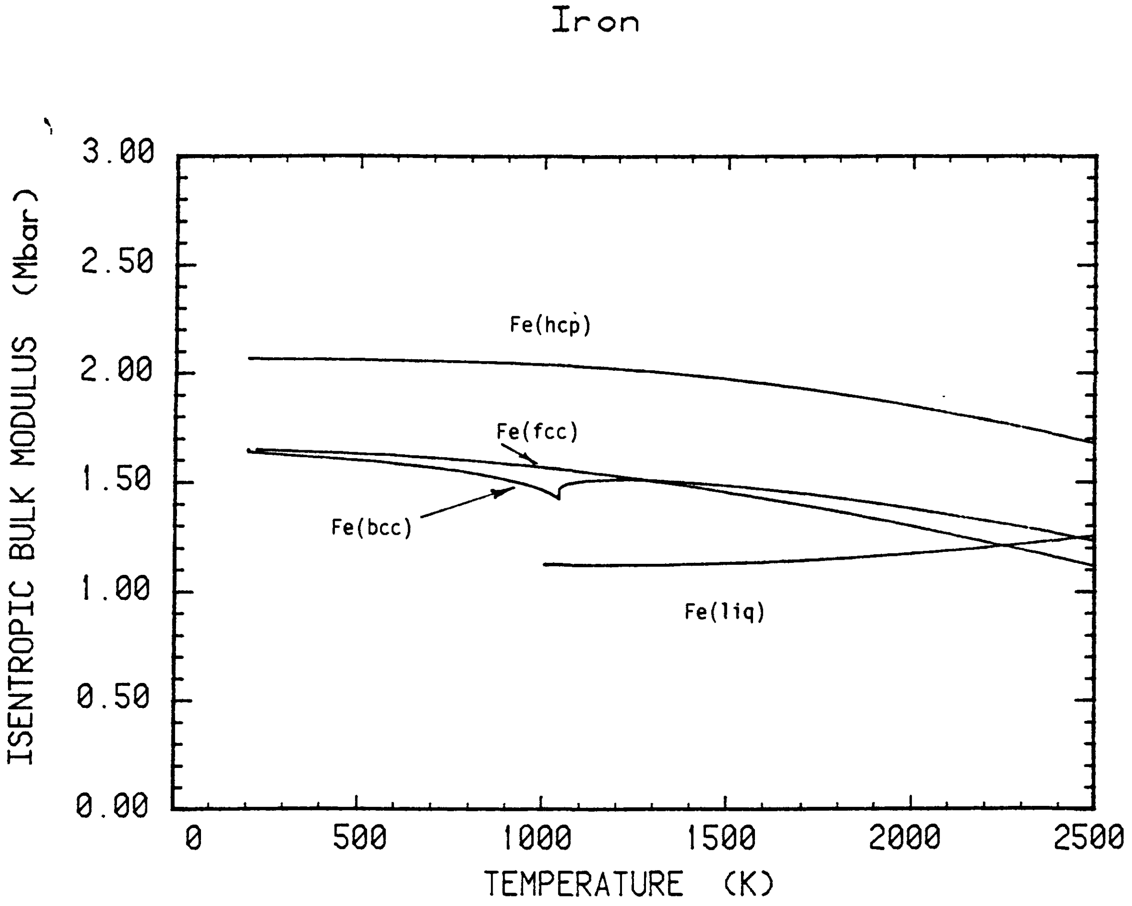


Figure 71. Plot of the calculated isentropic bulk modulus for the three solids and for Fe(liq).

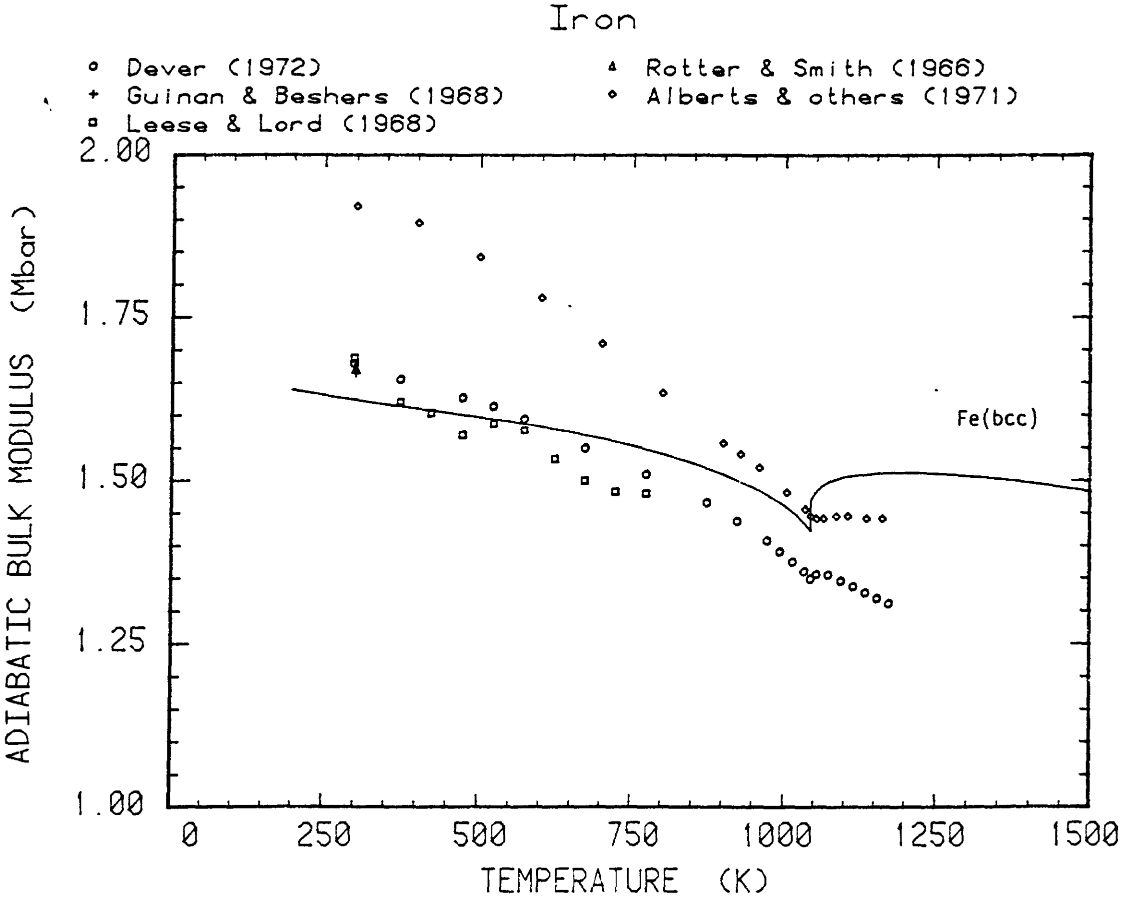


Figure 72. Comparison of the calculated isentropic bulk modulus for Fe(bcc) and the data calculated from elastic constants measured by Dever (1972), Guinan and Beshers (1968), Leese and Lord (1968), Rotter and Smith (1966), and Albert and others (1971).

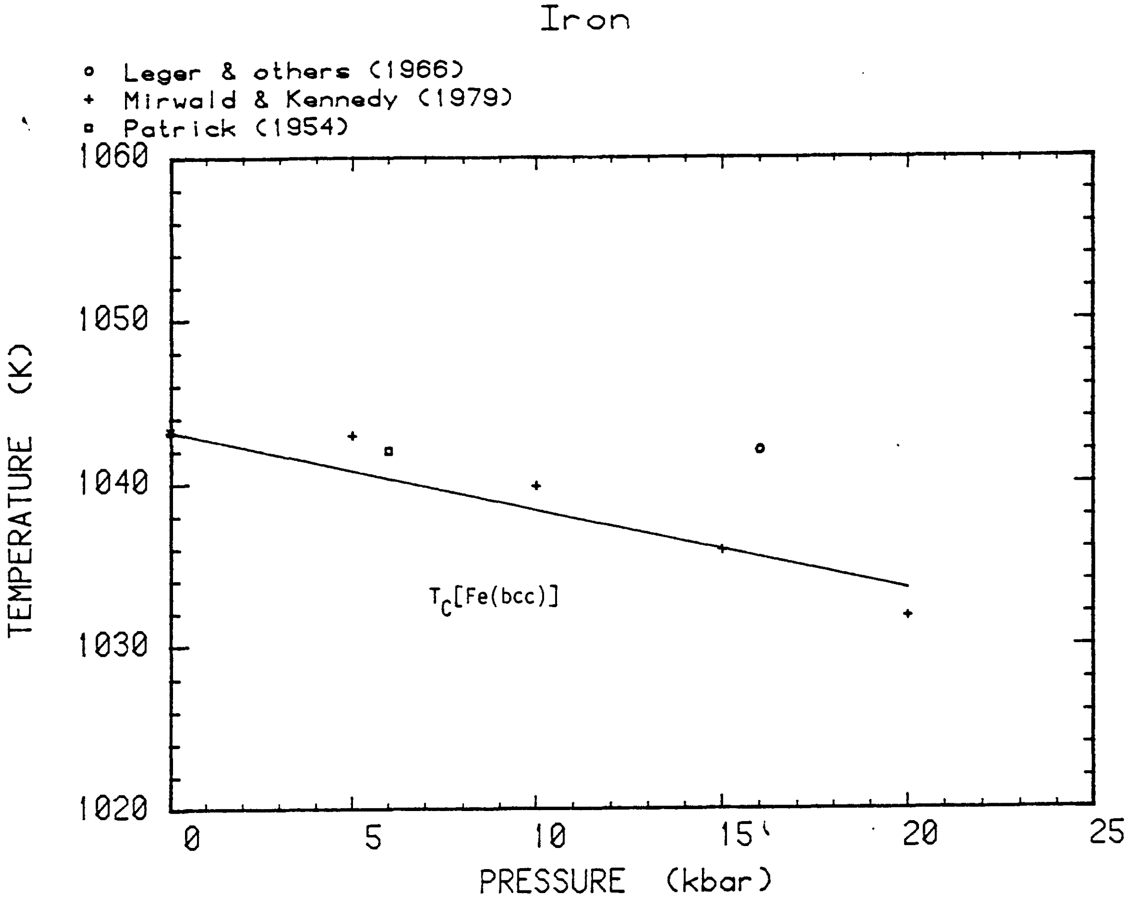


Figure 73. Comparison of the calculated critical temperature for Fe(bcc) as a function of pressure and the available experimental data.

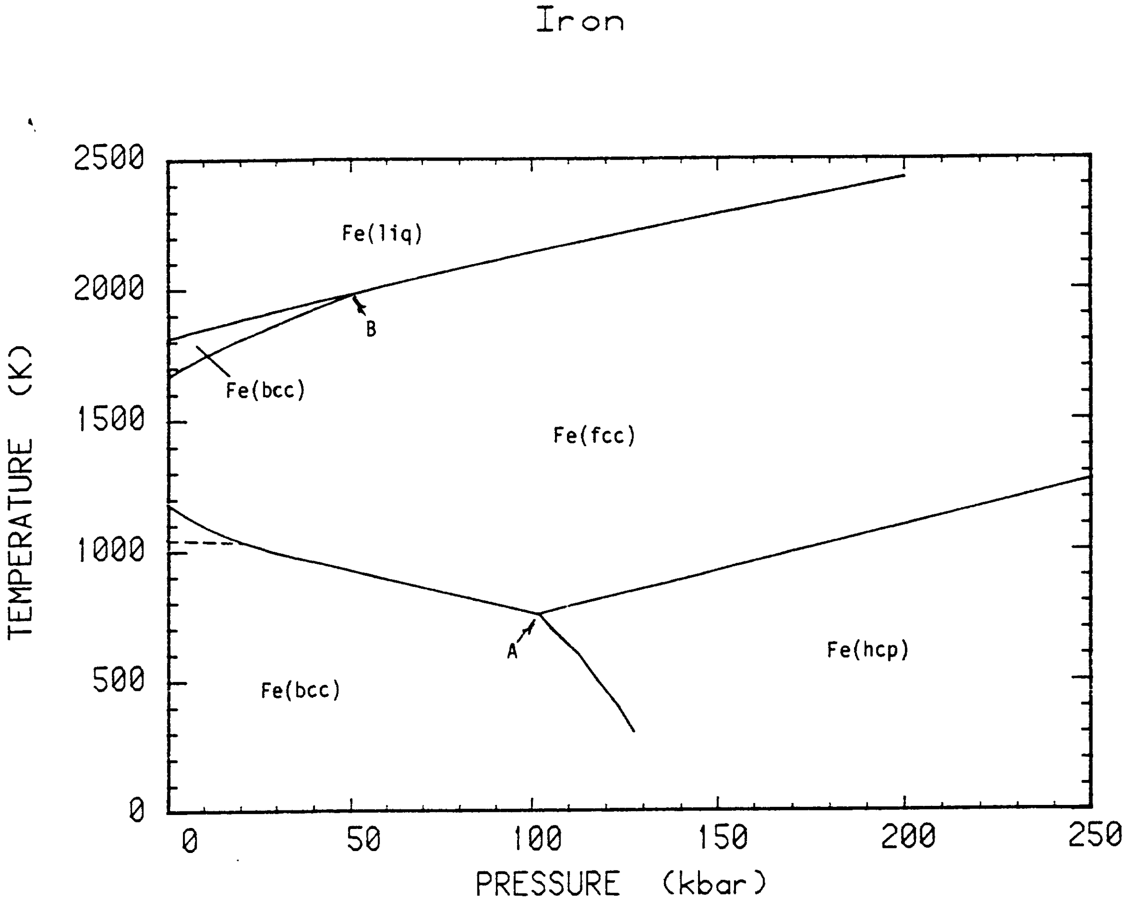


Figure 74. Plot of the calculated univariant reactions among the iron phases as a function of temperature and pressure. The dashed line shows the location of T(crit) for Fe(bcc).

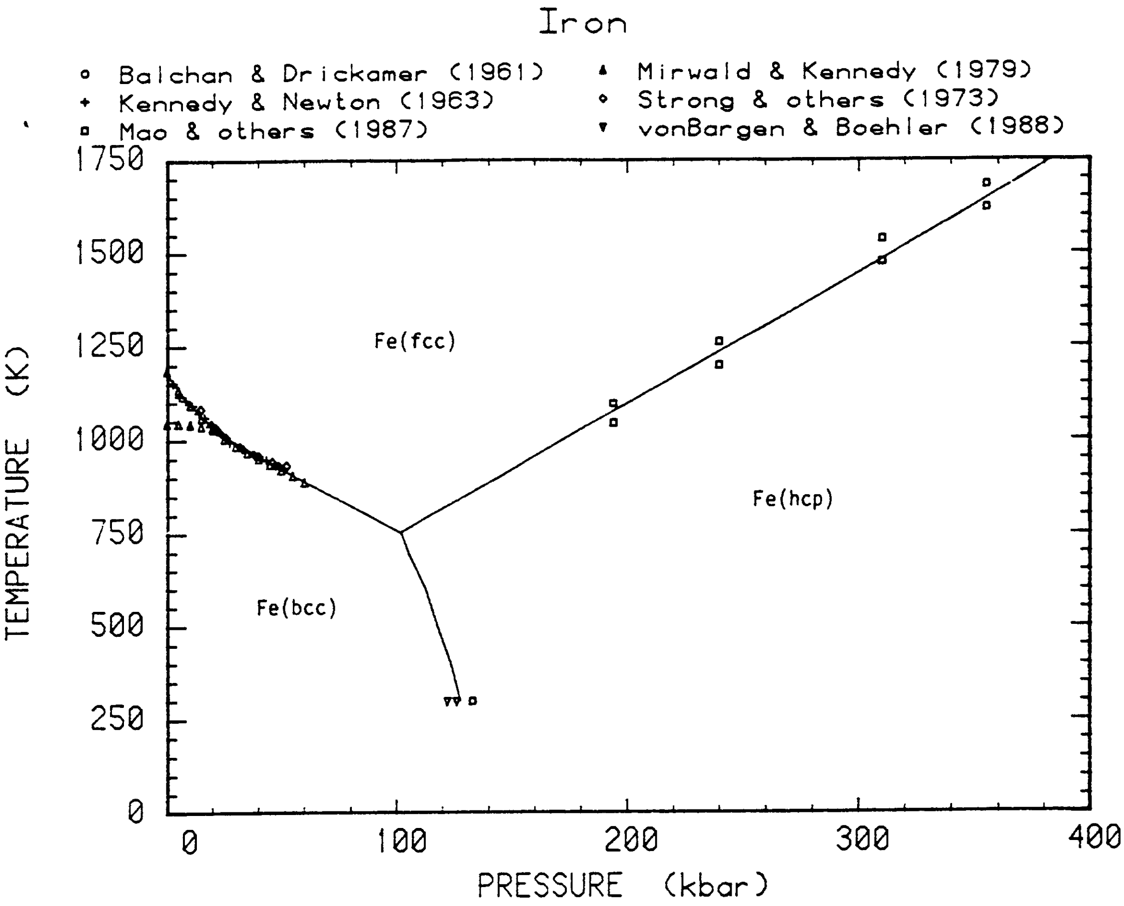
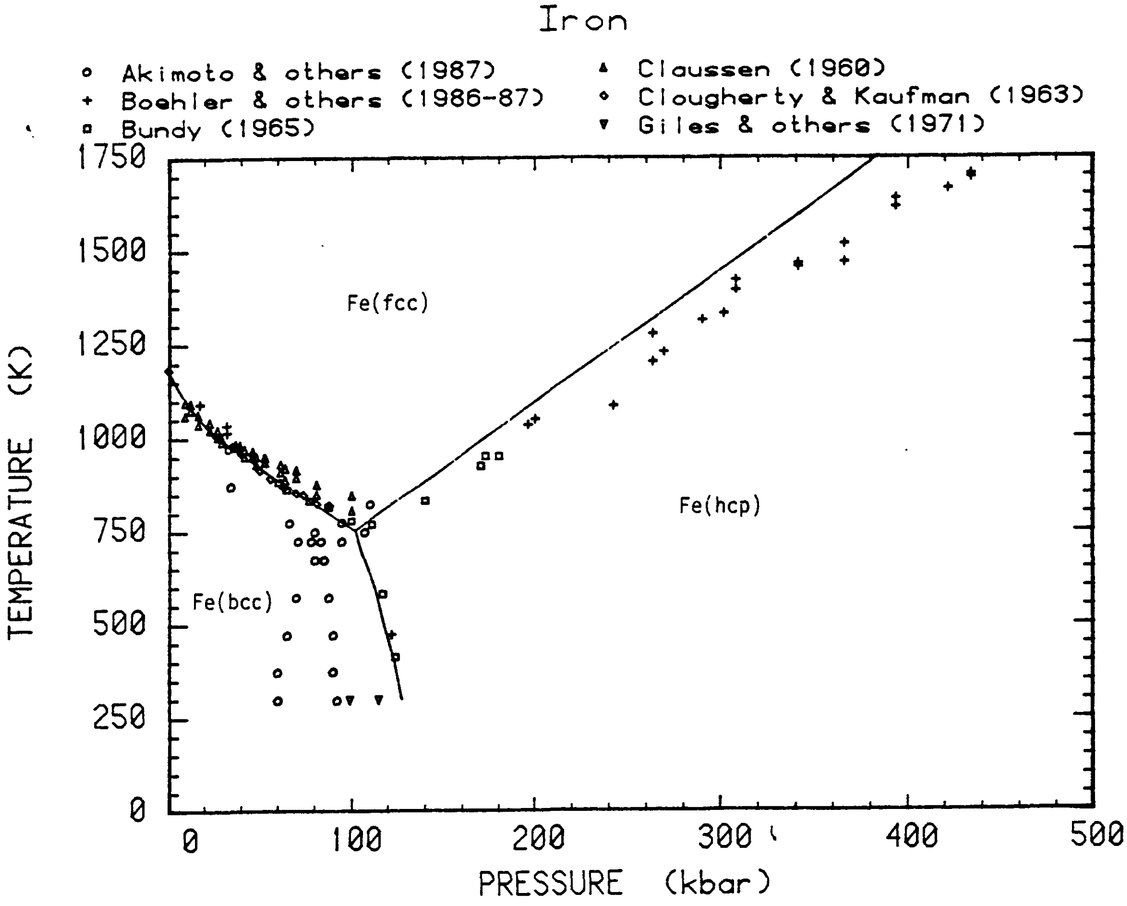
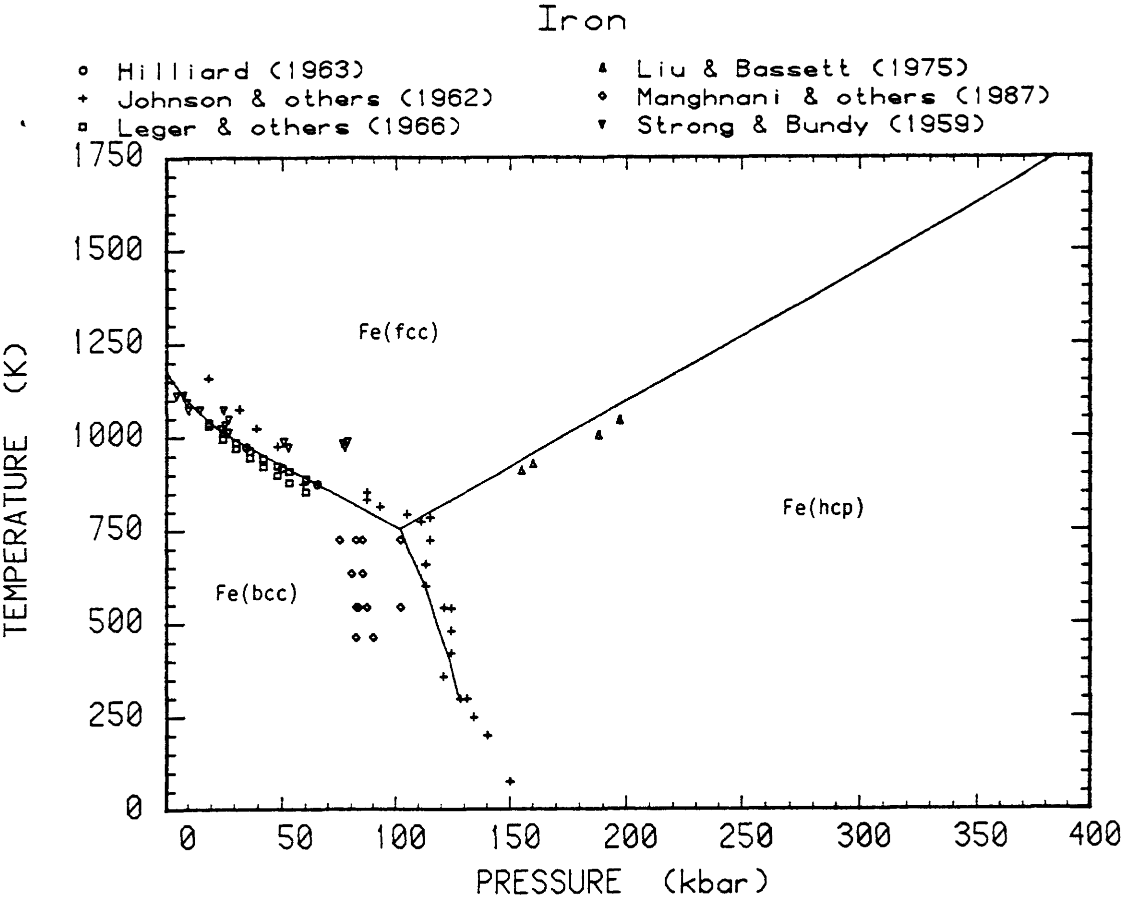


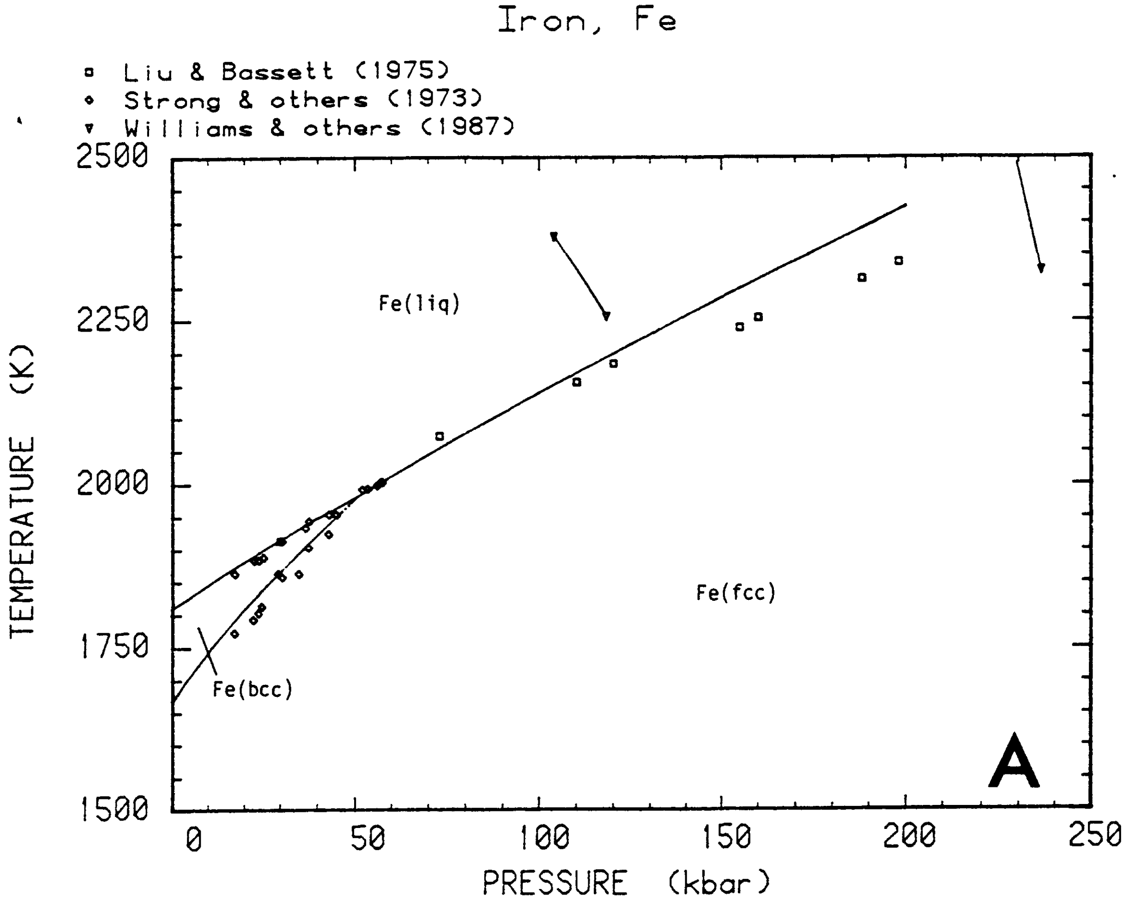
Figure 75. Comparison of the calculated univariant reactions associated with the invariant point A and the experimental data used in the evaluation.



Figue 76. Comparison of the calculated univariant reactions associated with the invariant point A and the data from the following sources that were not used in the evaluation: Akimoto and others (1987); Boehler (1986); Boehler and others (1986,1987); Bundy (1965); Claussen (1960); Clougherty and Kaufman (1963); and Giles and others (1971).

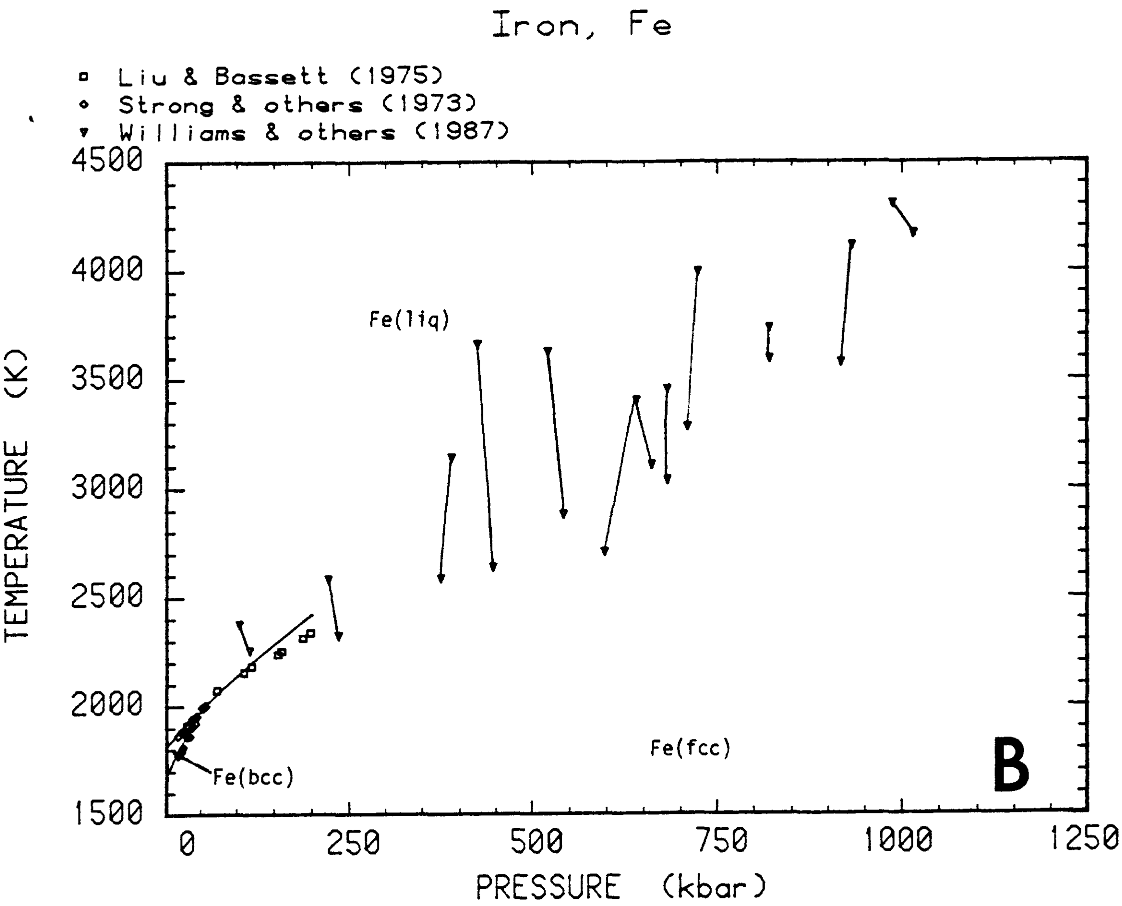


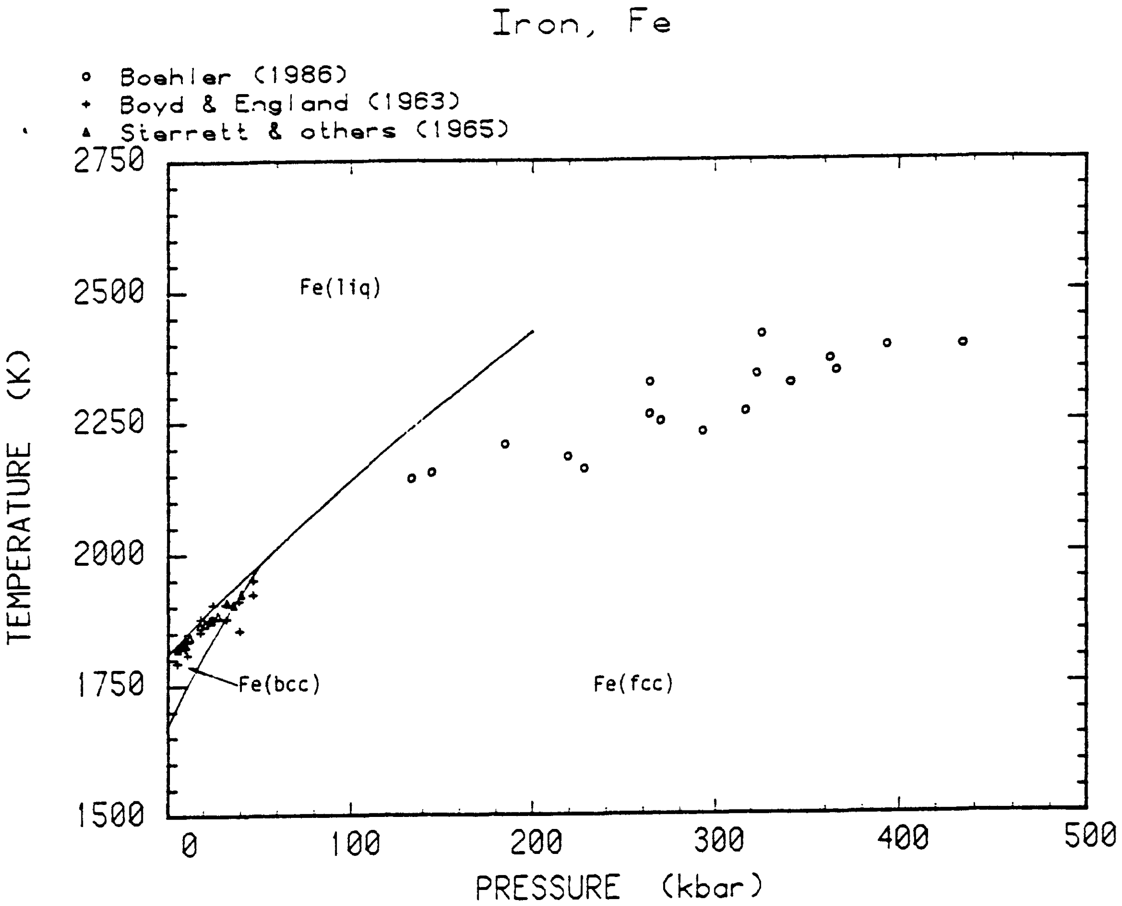
Figue 77. Comparison of the calculated univariant reactions associated with the invariant point A and the data from the following sources that were not used in the evaluation: Hilliard (1963); Johnson and others (1962); Leger and others (1966); Liu and Bassett (1975); Manghnani and others (1987); and Strong and Bundy (1959).



Figue 78. Comparison of the calculated univariant reactions associated with the invariant point B and the data from the following sources that were used in the evaluation: Liu and Bassett (1975); Strong and others (1973), and Williams and others (1987). Figure 78a shows the details around the triple point at A. Figure 78b is a replot of the data as a scale such that all the data of Williams and others (1987) could be shown.

(Figure 78b is on the next page.)


Iron, Fe
▫ Liu & Bassett (1975)
◦ Strong & others (1973)
▾ Williams & others (1987)
TEMPERATURE (K)
4500
4000
3500
3000
2500
2000
1500
PRESSURE (kbar)
0
250
500
750
1000
1250
Fe(liq)
Fe(fcc)
Fe(bcc)
B



Figue 79. Comparison of the calculated univariant reactions associated with the invariant poing B and the data from the following sources that were not used in the evaluation: Boehler (1986); Boyd and England (1963); and Sterrett and others (1965).

Table 1. Constants by phase for equations 1 through 29.

EQUATION	PHASE			
SYMBOL	Fe(bcc)	Fe(fcc)	Fe(hcp)	Fe(liq)
a_1	5.381856×10^{7}	1.897300×10^{8}	-----	-----
a_2	-1.075432×10^{6}	-3.252687×10^{6}	3.990575×10^{5}	-----
a_3	8.463703×10^{3}	2.501975×10^{4}	-1.116638×10^{4}	-----
a_4	-4.930500×10^{2}	-1.267098×10^{3}	7.820147×10^{2}	-5.106556×10^{2}
a_5	3.253110×10^{1}	4.588525×10^{1}	1.091042×10^{1}	5.519394×10^{1}
a_6	8.323558×10^{-3}	5.337877×10^{-3}	8.521542×10^{-3}	-----
a_7	-----	-----	-----	-----
a_8	-----	-----	-----	-----
a_9	-4.459718×10^{4}	-1.162952×10^{5}	3.992045×10^{4}	1.597746×10^{4}
a_{10}	-1.947307×10^{2}	-3.130002×10^{2}	2.111533×10^{1}	-3.381642×10^{2}
a_{11}	1043.2	67.0	-----	-----
a_{12}	-4.660776×10^{-6}	-----	-----	-----
a_{13}	1.610258×10^{1}	9.238051	-----	-----
a_{14}	1.149176×10^{1}	3.766899	-----	-----
j'	3	3	-----	-----
j''	-5	-5	-----	-----
n	15	3	-----	-----
b_1	6.706696×10^{-5}	7.060262×10^{-5}	6.717989×10^{-5}	7.085516×10^{-5}
b_2	-----	-----	-----	2.557665×10^{-8}
b_3	-5.041081×10^{-5}	5.720009×10^{-7}	-1.066327×10^{-5}	-----
b_4	1.676787×10^{6}	1.639222×10^{6}	2.042590×10^{6}	1.167751×10^{6}
b_5	-2.712230×10^{2}	-3.012328×10^{2}	-3.147723×10^{2}	-2.277294×10^{2}
b_6	7.014576	5.965451	4.143368	3.927332
b_7	6.808980	6.710926	6.525730	6.707135
b_8	650.0	650.0	650.0	-----

Table 2. Heat capacity of the iron polymorphs as a function of the absolute temperature.

Temperature (K)	Fe(bcc)	Fe(fcc)	Fe(hcp)	Fe(liq)
	----------------	J/(mol	K)	----------------
200	21.6054	24.8692	22.0561	---
225	22.7936	26.2268	23.2164	---
250	23.7427	27.2653	24.2192	---
273.15	24.4737	27.9908	25.0233	---
298.15	25.1543	28.5808	25.7776	---
300	25.2013	28.6180	25.8292	---
350	26.3563	29.3829	27.0471	---
400	27.3955	29.8506	27.9979	---
450	28.4174	30.1749	28.7661	---
500	29.4794	30.4346	29.4074	---
550	30.6192	30.6701	29.9592	---
600	31.8661	30.9017	30.4468	---
650	33.2480	31.1394	30.8880	---
700	34.7970	31.3875	31.2953	---
750	36.5553	31.6476	31.6777	---
800	38.5873	31.9198	32.0416	---
850	41.0011	32.2033	32.3920	---
900	44.0044	32.4971	32.7325	---
950	48.0826	32.7999	33.0659	---
975	50.9143	32.9544	33.2305	---
1000	54.8804	33.1108	33.3941	39.0456
1005	55.9081	33.1422	33.4267	39.0858
1010	57.0529	33.1738	33.4593	39.1257
1015	58.3414	33.2054	33.4918	39.1654
1020	59.8083	33.2371	33.5244	39.2047
1025	61.4988	33.2688	33.5568	39.2437
1030	63.4733	33.3006	33.5893	39.2825
1035	65.8120	33.3325	33.6217	39.3210
1040	68.6228	33.3644	33.6541	39.3592
1041	69.2536	33.3708	33.6606	39.3668
1042	69.9104	33.3772	33.6671	39.3744
1043	70.5946	33.3836	33.6736	39.3820
1043.2	70.7349	33.3849	33.6748	39.3835
1044	59.3301	33.3900	33.6800	39.3895
1045	58.5868	33.3964	33.6865	39.3971
1050	55.5458	33 4285	33.7189	39.4348
1060	51.6259	33.4927	33.7835	39.5093
1070	49.2067	33.5573	33 8480	39.5827
1080	47 5365	33.6220	33.9125	39.6552
1090	46.2907	33.6869	33.9769	39 7266
1100	45.3117	33.7521	34.0413	39.7971
1150	42.3708	34.0807	34.3624	40.1355
1184	41.2684	34.3066	34.5804	40.3533
1200	40.8829	34.4135	34.6829	40.4526
1300	39.5509	35.0892	35.3242	41.0309
1400	39.2110	35.7745	35.9684	41.5461
1500	39.3528	36.4661	36.6174	42.0089
1600	39.7657	37.1615	37.2722	42.4275
1665	40.1266	37.6145	37.7012	42.6792
1700	40.3429	37.8586	37.9333	42.8087
1800	41.0240	38.5561	38.6011	43.1577
1809	41.0891	38.6189	38.6615	43.1876
1900	41.7729	39.2529	39.2755	43.4787
2000	42.5669	39.9482	39.9565	43.7753
2200	44.2366	41.3323	41.3372	44.3067
2400	45.9654	42.7055	42.7416	44.7702
2600	47.7216	44.0665	44.1673	45.1792
2800	49.4898	45.4148	45.6123	45.5435
3000	51.2621	46.7505	47.0748	45.8707

Uncertainties in Functions

298.15	0.065	1 21	0.611	---
500	0.066	0.89	1.33	---
1000	0.26	0.35	1.36	1.65
1043.2	0.44	---	---	---
1500	0.138	0.26	1.85	1.00
2000	0.55	0.79	2.5	1.00
3000	2.00	2.4	3.8	1.34

Table 3. Incremental enthalpy of the iron polymorphs as a function of the absolute temperature.

Temperature (K)	Fe(bcc)	Fe(fcc)	Fe(hcp)	Fe(liq)
	J/mol			
200	-2317.	3858.	3233.	---
225	-1761.	4497.	3800.	---
250	-1179.	5166.	4393.	---
273.15	-621.	5806.	4963.	---
298.15	0.	6514.	5598.	---
300	47.	6567.	5646.	---
350	1336.	8018.	6969.	---
400	2680.	9500.	8346.	---
450	4076.	11001.	9766.	---
500	5523.	12517.	11221.	---
550	7025.	14044.	12705.	---
600	8586.	15583.	14216.	---
650	10214.	17134.	15749.	---
700	11914.	18698.	17304.	---
750	13697.	20273.	18878.	---
800	15574.	21863	20471.	---
850	17562.	23466.	22082.	---
900	19684.	25083.	23710.	---
950	21980.	26715.	25355.	---
975	23216.	27537.	26184.	---
1000	24535.	28363.	27017.	38875.
1005	24812.	28529.	27184.	39070.
1010	25094.	28695.	27351.	39266.
1015	25382.	28861.	27519.	39461.
1020	25678.	29027.	27686.	39657.
1025	25981.	29193.	27854.	39853.
1030	26293.	29359.	28022.	40050.
1035	26616.	29526.	28190.	40246.
1040	26952.	29693	28358.	40443.
1041	27021.	29726.	28392.	40482.
1042	27091.	29759.	28425.	40522.
1043	27161.	29793.	28459.	40561.
1043.2	27175.	29799.	28466.	40569.
1044	27223.	29826.	28493.	40600.
1045	27282.	29860.	28526.	40640.
1050	27567.	30027.	28695.	40837.
1060	28101.	30361.	29032.	41232.
1070	28604.	30697.	29370.	41627.
1080	29087.	31032.	29709.	42023.
1090	29556.	31369.	30049.	42420.
1100	30014.	31706.	30389.	42818.
1150	32196.	33402.	32099.	44816.
1184	33617.	34565.	33271.	46185.
1200	34274.	35114.	33825.	46831.
1300	38284.	38589.	37325.	50906.
1400	42216.	42132.	40890.	55035.
1500	46142.	45744.	44519.	59213
1600	50096.	49426.	48214.	63435.
1665	52692.	51856.	50650.	66201.
1700	54100.	53177.	51974.	67697.
1800	58168.	56998.	55801.	71996.
1809	58537.	57345.	56148.	72385.
1900	62307.	60888.	59694.	76328.
2000	66524.	64848.	63656.	80691.
2200	75203.	72976.	71785.	89500.
2400	84222.	81380.	80192.	98409.
2600	93591.	90058.	88883.	107405.
2800	103312.	99006.	97861.	116478.
3000	113387.	108223.	107129.	125620.

Uncertainties in Functions

298.15	0.	0.	0.	---
500	13.	196.	212.	---
1000	28.	470.	830.	2180.
1043.2	40	---	---	---
1500	42.	500.	1400.	2720.
2000	150.	460.	2200.	3000.
3000	1330.	1700.	4900.	3100.

Table 4. Entropy of the iron polymorphs as a function of the absolute temperature.

Temperature (K)	Fe(bcc)	Fe(fcc)	Fe(hcp)	Fe(liq)
	J/(mol K)			
200	17.9417	22.4399	20.8766	---
225	20.5579	25.4507	23.5430	---
250	23.0103	28.2704	26.0423	---
273.15	25.1457	30.7181	28.2231	---
298.15	27.3190	33.1961	30.4479	---
300	27.4748	33.3730	30.6075	---
350	31.4487	37.8472	34.6846	---
400	35.0366	41.8035	38.3608	---
450	38.3222	45.3391	41.7043	---
500	41.3707	48.5321	44.7692	---
550	44.2331	51.4440	47.5985	---
600	46.9499	54.1225	50.2266	---
650	49.5541	56.6053	52.6814	---
700	52.0736	58.9220	54.9855	---
750	54.5329	61.0963	57.1578	---
800	56.9553	63.1474	59.2139	---
850	59.3647	65.0910	61.1670	---
900	61.7897	66.9400	63.0282	---
950	64.2714	68.7051	64.8069	---
975	65.5553	69.5591	65.6679	---
1000	66.8910	70.3954	66.5113	75.3987
1005	67.1672	70.5606	66.6779	75.5936
1010	67.4475	70.7251	66.8439	75.7876
1015	67.7323	70.8890	67.0092	75.9810
1020	68.0225	71.0523	67.1739	76.1735
1025	68.3190	71.2149	67.3379	76.3653
1030	68 6230	71.3769	67.5013	76.5564
1035	68.9358	71.5382	67.6640	76.7467
1040	69.2595	71.6989	67.8261	76.9363
1041	69.3258	71.7310	67.8585	76.9741
1042	69.3926	71.7630	67.8908	77.0119
1043	69.4600	71.7950	67.9231	77.0497
1043.2	69.4735	71.8014	67.9295	77.0573
1044	69.5193	71.8270	67.9554	77.0874
1045	69.5757	71.8590	67.9876	77.1252
1050	69.8477	72.0185	68.1485	77.3133
1060	70.3540	72.3357	68.4684	77.6875
1070	70.8266	72.6505	68.7859	78.0588
1080	71.2762	72.9629	69.1011	78.4273
1090	71.7083	73.2731	69.4139	78.7931
1100	72.1264	73.5810	69.7245	79.1563
1150	74.0672	75.0886	71 2448	80.9329
1184	75.2846	76.0849	72.2492	82.1055
1200	75.8359	76.5461	72.7140	82.6478
1300	79.0459	79.3272	75.5155	85.9090
1400	81.9605	81.9527	78.1568	88.9690
1500	84.6686	84.4444	80.6605	91.8514
1600	87.2205	86.8201	83.0446	94.5762
1665	88.8110	88.3088	84.5373	96.2707
1700	89.6479	89.0939	85.3240	97.1599
1800	91.9728	91.2776	87.5111	99.6168
1809	92.1775	91.4700	87.7038	99.8322
1900	94.2106	93.3808	89.6162	101.9590
2000	96.3733	95.4119	91.6480	104.1970
2200	100.5080	99.2844	95.5208	108.3950
2400	104.4310	102.9400	99.1777	112.2700
2600	108.1790	106.4120	102.6550	115.8700
2800	111.7810	109.7270	105.9810	119.2320
3000	115.2550	112.9060	109.1780	122.3850

Uncertainties in Functions

298.15	0.002	0.913	1.150	---
500	0.034	0.500	0.910	---
1000	0.035	0.044	1.130	0.700
1043.2	0.042	---	---	---
1500	0.029	0.035	1.500	0.236
2000	0.088	0.163	1.900	0.078
3000	0.550	0.730	2.800	0.500

Table 5. Enthalpy difference for the iron polymorphs as a function of the absolute temperature.

Temperature (K)	Fe(bcc)= Fe(fcc)	Fe(bcc)= Fe(hcp)	Fe(bcc)= Fe(liq)	Fe(fcc)= Fe(hcp)	Fe(fcc)= Fe(liq)	Fe(hcp)= Fe(liq)
	J/mol					
200	6174.	5550.	---	-624.	---	---
225	6258.	5561.	---	-697.	---	---
250	6345.	5572.	---	-773.	---	---
273.15	6427.	5584.	---	-843.	---	---
298.15	6514.	5598.	---	-915.	---	---
300	6520.	5599.	---	-921.	---	---
350	6682.	5633.	---	-1049.	---	---
400	6820.	5666.	---	-1154.	---	---
450	6926.	5690.	---	-1235.	---	---
500	6994.	5698.	---	-1296.	---	---
550	7019.	5680.	---	-1339.	---	---
600	6997.	5629.	---	-1368.	---	---
650	6921.	5536.	---	-1385.	---	---
700	6784.	5390.	---	-1394.	---	---
750	6577.	5181.	---	-1395.	---	---
800	6288.	4897.	---	-1391.	---	---
850	5904.	4520.	---	-1383.	---	---
900	5399.	4027	---	-1373.	---	---
950	4736.	3376.	---	-1360.	---	---
975	4322.	2968.	---	-1353.	---	---
1000	3828.	2482.	14340.	-1346.	10512.	65892.
1005	3717.	2372.	14258.	-1345.	10541.	66254.
1010	3601.	2257.	14172.	-1343.	10571.	66617.
1015	3478.	2136.	14079.	-1342.	10601.	66980.
1020	3349.	2008.	13980.	-1341.	10631.	67343.
1025	3212.	1873.	13872.	-1339.	10660.	67707.
1030	3066.	1728.	13757.	-1338.	10690.	68071.
1035	2910.	1573.	13630	-1336.	10720.	68436.
1040	2741.	1406.	13491.	-1335.	10750.	68801.
1041	2705.	1371.	13461.	-1334.	10756.	68874.
1042	2669.	1335.	13431.	-1334	10762.	68947.
1043	2632.	1298.	13400.	-1334.	10768.	69020.
1043.2	2624	1291.	13394.	-1334.	10769.	69035.
1044	2603.	1270.	13378.	-1334.	10774.	69093
1045	2578.	1245.	13358.	-1333.	10780.	69166.
1050	2460.	1128.	13270.	-1332.	10810.	69532.
1060	2261.	932.	13131.	-1329.	10870.	70264.
1070	2092.	766.	13023.	-1326.	10931.	70997.
1080	1945.	622.	12936.	-1323	10991.	71732.
1090	1813.	493.	12864.	-1320.	11051.	72469.
1100	1692.	375.	12804.	-1317.	11112.	73207.
1150	1206.	-98.	12620.	-1303.	11414.	76915.
1184	947.	-346.	12568.	-1294.	11620.	79455.
1200	840.	-449.	12557.	-1289.	11717.	80656.
1300	306.	-958.	12622.	-1264.	12316.	88231.
1400	-84.	-1326.	12819.	-1242.	12903.	95925.
1500	-397.	-1622.	13072.	-1225.	13469.	103732.
1600	-670.	-1882.	13340.	-1212.	14010.	111649.
1665	-836.	-2042.	13509.	-1206.	14345.	116852.
1700	-923.	-2126.	13597.	-1203.	14521.	119671.
1800	-1170.	-2367.	13828.	-1197.	14999.	127796.
1809	-1193.	-2389.	13847.	-1197.	15040.	128533.
1900	-1419.	-2613	14021.	-1194.	15440.	136022.
2000	-1676.	-2868.	14167.	-1192.	15843.	144347.
2200	-2227.	-3418.	14298.	-1191.	16524.	161285.
2400	-2842.	-4030.	14187.	-1188.	17029.	178601.
2600	-3533.	-4708.	13814.	-1175.	17347.	196288.
2800	-4306.	-5451.	13166.	-1145.	17472.	214338.
3000	-5164.	-6258.	12233.	-1094.	17397.	232749.

Uncertainties in Functions

298.15	495.	435.	---	480.	---	---
500	340.	360.	---	320.	---	---
1000	44.	710.	950.	700.	950.	1200.
1043.2	42.	750.	900.	---	---	---
1500	18	1310.	400.	1300.	400.	1370.
2000	310.	2180.	210.	2200.	300.	2200.
3000	2130.	5000.	1800.	5200.	2100.	5000.

Table 6. The enthalpies (J/mol) of the high-temperature transformations as found in this optimization and as reported by various sources Data flagged with an asterisk (*) were explicitly used in this optimization. Other data were either givan zero weight or were implicit in studies of incremental enthalpy used for the optimization.

SOURCE	REACTIONS		
	Fe(bcc)=Fe(fcc) T=1184 K	Fe(fcc)=Fe(bcc) T=1665 K	Fe(bcc)=Fe(liq) T=1809 K
This Research	947	835	13,847
Agren (1979)	1,011	825	13,807
Anderson and Hultgren (1962)	941	---	---
Austin (1932)	912	1,046	15,328
Bendick and Pepperhoff (1982)	820	850	---
Braun and Kohlhaas (1965)	910	865	---
Cezairlyan and McClure (1974)	---	890	---
Chase and others (1985)	900	837	13,807
Chuang and others (1985)	937	821	---
Darken and Smith (1951)	900	690	15,355
Dench and Kubachewski (1963)	900	837	---
Esser and Baerlecken (1941)	918	---	---
Fernandez Guillermet and Gustafson (1985)	1,013	826	13 807
Ferrier (1962)	---	---	13.807*
Ferrier and Olette (1962)	---	1.100	13,773
Hultgren and others (1973)	900	836	13 807
Johansson (1937)	1.188	441	---
Klinkhardt (1927)	902	---	---
Margrave (1975)	---	---	14.100
Morris and others (1966)	---	---	13.799
Orr and Chipman (1967)	900	837	13,807
Pattison and Willows (1956)	---	865	15,306
Rogez and LeCoze (1980)	901	---	---
Sale (1970)	925*	---	---
Schuermann and Kaiser (1981)	954	770	14 390
Schuermann and Neubert (1979)	900	819	14.403
Smith (1946)	900	---	---
Treverton and Margrave (1971)	---	---	13.836*
Tsuchiya and others (1971)	900	837	---
Vollmer and others (1966)	---	---	14.400
Wallace and others (1960)	911	---	---
Zuitoff (1938)	748	514	---

Table 7. Gibbs energy difference for the iron polymorphs as a function of the absolute temperature.

Temperature (K)	Fe(bcc)= Fe(fcc)	Fe(bcc)= Fe(hcp)	Fe(bcc)= Fe(liq)	Fe(fcc)= Fe(hcp)	Fe(fcc)= Fe(liq)	Fe(hcp)= Fe(liq)
	J/mol					
200	5275	4963	---	-312.	---	---
225	5157.	4889.	---	-268.	---	---
250	5030.	4814.	---	-216.	---	---
273.15	4905.	4743.	---	-162.	---	---
298.15	4762.	4665.	---	-96.	---	---
300	4751.	4660.	---	-91.	---	---
350	4443.	4500.	---	58.	---	---
400	4113.	4336.	---	223.	---	---
450	3768.	4169.	---	401.	---	---
500	3413.	3999.	---	586.	---	---
550	3053.	3829.	---	776.	---	---
600	2693.	3663.	---	970.	---	---
650	2337.	3503.	---	1165.	---	---
700	1990.	3352.	---	1362.	---	---
750	1654.	3213.	---	1559	---	---
800	1335.	3090.	---	1756.	---	---
850	1036.	2988.	---	1952.	---	---
900	764.	2912.	---	2148.	---	---
950	524.	2867.	---	2343.	---	---
975	418.	2859.	---	2441.	---	---
1000	324.	2862.	5832.	2538	5508.	2970.
1005	307	2864.	5790.	2557.	5483.	2926.
1010	290.	2867.	5748.	2577.	5458.	2881.
1015	274.	2870.	5706.	2596.	5432.	2836.
1020	259.	2874.	5665.	2615.	5407.	2791.
1025	244.	2879.	5625.	2635.	5381.	2746.
1030	230.	2884.	5585.	2654.	5355.	2701.
1035	216.	2890.	5546.	2674.	5329.	2656.
1040	204.	2897	5507.	2693	5303.	2610.
1041	201.	2898.	5499.	2697.	5298.	2601.
1042	199.	2899.	5492.	2701.	5293.	2592.
1043	196.	2901.	5484.	2705.	5288.	2583.
1043.2	196.	2901.	5483.	2705.	5287.	2581.
1044	194.	2903.	5476.	2708.	5282.	2574.
1045	192.	2904.	5469.	2712	5277.	2565.
1050	181.	2912.	5431.	2732.	5251.	2519.
1060	160.	2930.	5357.	2770.	5197.	2427.
1070	141.	2950.	5285.	2809.	5144.	2335.
1080	123.	2971.	5213.	2848.	5089.	2242
1090	107.	2993.	5142.	2886.	5034.	2148.
1100	92.	3017.	5071.	2925.	4979.	2054.
1150	31.	3148.	4724.	3117.	4693.	1576.
1184	0.	3248.	4492.	3248.	4492.	1244.
1200	-12.	3297.	4383.	3309.	4395.	1085.
1300	-60.	3631.	3700.	3691.	3760.	69.
1400	-73.	3999.	3007.	4072.	3080.	-992.
1500	-61.	4390.	2297.	4451.	2358.	-2092.
1600	-29.	4799.	1570.	4829.	1600.	-3229.
1665	0.	5074	1089.	5074.	1089.	-3985.
1700	18.	5224.	827.	5206.	808.	-4398.
1800	81.	5664.	69.	5583.	-12.	-5595.
1809	87.	5704.	0.	5617.	-87.	-5704.
1900	157.	6117.	-701.	5959.	-858.	-6818.
2000	247.	6583.	-1480.	6336.	-1727.	-8062.
2200	465.	7554.	-3053.	7088.	-3518.	-10607.
2400	737.	8578.	-4627.	7841.	-5364.	-13205.
2600	1062.	9655.	-6182.	8593.	-7244.	-15837.
2800	1444.	10788.	-7697.	9343.	-9142.	-18485.
3000	1885.	11976.	-9157.	10091.	-11041.	-21132.

Uncertainties in Functions

298.15	230.	210.	---	50.	---	---
500	100.	260.	---	200.	---	---
1000	5.	630.	260.	630.	260.	680.
1043.2	4.	670.	230.	---	---	---
1500	5.	1200.	47.	1200.	47.	1200.
2000	35.	1950.	16	1960.	34.	1950.
3000	510.	4050.	400.	4100.	510	4100.

Table 8. Molar Volume of the iron polymorphs as a function of the absolute temperature.

Temperature (K)	Fe(bcc)	Fe(fcc)	Fe(hcp)	Fe(liq)
	cm^3/mol			
200	7.0692	6.8045	6.6478	---
225	7.0746	6.8166	6.6577	---
250	7.0802	6.8287	6.6676	---
273.15	7.0857	6.8399	6.6769	---
298.15	7.0917	6.8521	6.6870	---
300	7.0922	6.8530	6.6877	---
350	7.1050	6.8773	6.7081	---
400	7.1187	6.9018	6.7286	---
450	7.1330	6.9263	6.7494	---
500	7.1479	6.9509	6.7704	---
550	7.1633	6.9755	6.7915	---
600	7.1793	7.0003	6.8129	---
650	7.1956	7.0251	6.8344	---
700	7.2123	7.0500	6.8561	---
750	7.2293	7.0750	6.8780	---
800	7.2464	7.1001	6.9000	---
850	7.2636	7.1253	6.9222	---
900	7.2807	7.1505	6.9445	---
950	7.2975	7.1759	6.9670	---
975	7.3056	7.1886	6.9783	---
1000	7.3136	7.2013	6.9896	7.2923
1005	7.3151	7.2038	6.9919	7.2958
1010	7.3166	7.2064	6.9941	7.2993
1015	7.3181	7.2089	6.9964	7.3028
1020	7.3196	7.2115	6.9987	7.3064
1025	7.3210	7.2140	7.0009	7.3099
1030	7.3224	7.2166	7.0032	7.3135
1035	7.3237	7.2191	7.0055	7.3170
1040	7.3250	7.2217	7.0078	7.3206
1041	7.3253	7.2222	7.0082	7.3213
1042	7.3255	7.2227	7.0087	7.3220
1043	7.3258	7.2232	7.0091	7.3227
1043.2	7.3258	7.2233	7.0092	7.3229
1044	7.3261	7.2237	7.0096	7.3235
1045	7.3264	7.2242	7.0101	7.3242
1050	7.3279	7.2268	7.0123	7.3277
1060	7.3312	7.2319	7.0169	7.3349
1070	7.3346	7.2370	7.0215	7.3421
1080	7.3381	7.2421	7.0260	7.3494
1090	7.3417	7.2473	7.0306	7.3566
1100	7.3454	7.2524	7.0352	7.3639
1150	7.3646	7.2781	7.0582	7.4006
1184	7.3782	7.2956	7.0739	7.4260
1200	7.3847	7.3038	7.0813	7.4381
1300	7.4268	7.3557	7.1280	7.5150
1400	7.4708	7.4078	7.1750	7.5946
1500	7.5161	7.4604	7.2226	7.6770
1600	7.5627	7.5133	7.2705	7.7623
1665	7.5935	7.5478	7.3020	7.8193
1700	7.6102	7.5665	7.3189	7.8506
1800	7.6587	7.6202	7.3677	7.9418
1809	7.6631	7.6250	7.3721	7.9502
1900	7.7079	7.6742	7.4170	8.0362
2000	7.7578	7.7286	7.4665	8.1339
2200	7.8597	7.8385	7.5669	8.3391
2400	7.9638	7.9500	7.6688	8.5582
2600	8.0700	8.0631	7.7722	8.7920
2800	8.1781	8.1778	7.8770	9.0415
3000	8.2881	8.2941	7.9834	9.3076

Uncertainties in Functions

Temperature (K)	Fe(bcc)	Fe(fcc)	Fe(hcp)	Fe(liq)
298.15	0.001	0.061	0.004	---
500	0.001	0.036	0.010	---
1000	0.003	0.005	0.030	0.064
1043.2	0.003	---	---	---
1500	0.006	0.002	0.060	0.023
2000	0.009	0.010	0.100	0.007
3000	0.018	0.048	0.200	0.060

Table 9. Sources of data on the density of liquid Fe. Data from citations flagged with an asterisk (*) were used in this optimization.

SOURCE	TEMPERATURE K	MAXIMUM ERROR cm /mol	AVERAGE ERROR cm /mol
* Grosse and Kirschenbaum (1963)	1812.3160	0.008,0.05	----
Ivakhnenko (1979)	1813-2073	0.09	0.06
* Kirschenbaum and Cahill (1962)	1805-2500	0.02	0.02
* Saito and others (1969)	1809-2423	0.01	0.01
* Saito and others (1970)	2073-2473	0.006	0 004
* Watanabe and others (1981)	1809-1923	0.01	0.01

Table 10. Cubic expansion coefficient of the iron polymorphs as a function of the absolute temperature.

Temperature (K)	Fe(bcc)	Fe(fcc)	Fe(hcp)	Fe(liq)
	10^{-6} K^{-1}			
200	29.9332	71.0231	59 3409	---
225	31.2999	71.0073	59.6367	---
250	32.6061	70.9920	59.9213	---
273.15	33.7626	70.9784	60.1752	---
298.15	34.9553	70.9642	60.4395	---
300	35.0413	70.9632	60.4587	---
350	37.2471	70.9365	60.9563	---
400	39.2307	70.9117	61.4171	---
450	40.9980	70.8889	61.8438	---
500	42.5537	70.8677	62.2389	---
550	43.9007	70.8480	62.6047	---
600	45.0396	70.8299	62.9434	---
650	45.9679	70.8130	63.2571	---
700	46.6776	70.7975	63.5475	---
750	47.1523	70.7830	63.8165	---
800	47.3610	70.7697	64.0655	---
850	47.2437	70.7573	64.2961	---
900	46.6768	70.7459	64.5096	---
950	45.3603	70.7353	64.7073	---
975	44.1763	70.7302	64.8006	---
1000	42.2586	70.7254	64.8904	96.4318
1005	41.7247	70.7245	64.9079	96.5597
1010	41.1160	70.7236	64.9253	96.6876
1015	40.4155	70.7226	64.9426	96.8155
1020	39.6014	70.7217	64.9597	96.9433
1025	38.6448	70.7208	64.9768	97.0712
1030	37.5075	70.7199	64.9936	97.1991
1035	36.1384	70.7190	65.0104	97.3270
1040	34.4693	70.7181	65.0270	97.4549
1041	34.0918	70.7179	65.0303	97.4805
1042	33.6978	70.7177	65.0336	97.5060
1043	33.2864	70.7176	65.0369	97.5316
1043.2	33.2020	70.7175	65.0376	97.5367
1044	40.4765	70.7174	65.0402	97.5572
1045	40.9727	70.7172	65.0435	97.5828
1050	43.0228	70.7163	65.0599	97.7106
1060	45.7431	70.7146	65.0922	97.9664
1070	47.5042	70.7129	65.1241	98.2222
1080	48.7851	70.7112	65.1555	98.4779
1090	49.7928	70.7095	65.1864	98.7337
1100	50.6277	70.7079	65.2168	98.9895
1150	53.5185	70.7001	65.3622	100.2680
1184	54 8786	70.6952	65.4548	101.1380
1200	55.4250	70.6929	65.4968	101.5470
1300	58.0378	70.6800	65.7368	104.1050
1400	59.8439	70.6690	65.9426	106.6620
1500	61.1960	70.6595	66.1190	109.2200
1600	62.2505	70.6514	66.2703	111.7780
1665	62.8188	70.6468	66.3568	113.4400
1700	63.0938	70.6445	66.4000	114.3350
1800	63.7796	70.6385	66.5112	116.8930
1809	63.8349	70.6380	66.5204	117.1230
1900	64.3441	70.6334	66.6065	119 4510
2000	64.8127	70.6290	66.6883	122.0080
2200	65.5330	70.6220	66.8185	127.1240
2400	66.0442	70.6169	66.9142	132.2390
2600	66.4105	70.6131	66.9846	137.3540
2800	66.6746	70.6103	67.0363	142.4700
3000	66.8655	70.6083	67.0743	147.5850

Table 11. Isothermal compressibility of the iron polymorphs as a function of the absolute temperature.

Temperature (K)	Fe(bcc)	Fe(fcc)	Fe(hcp)	Fe(liq)
	Mbar^{-1}			
200	0.6163	0.6333	0.5051	---
225	0.6189	0.6364	0.5072	---
250	0.6215	0.6394	0.5092	---
273.15	0.6239	0.6423	0.5111	---
298.15	0.6266	0.6454	0.5132	---
300	0.6268	0.6456	0.5133	---
350	0.6322	0.6520	0.5175	---
400	0.6376	0.6584	0.5217	---
450	0.6432	0.6650	0.5261	---
500	0.6489	0.6718	0.5304	---
550	0.6546	0.6786	0.5349	---
600	0.6605	0.6856	0.5395	---
650	0.6664	0.6928	0.5441	---
700	0.6725	0.7001	0.5488	---
750	0.6787	0.7076	0.5536	---
800	0.6850	0.7152	0.5584	---
850	0.6914	0.7230	0.5634	---
900	0.6980	0.7309	0.5684	---
950	0.7047	0.7391	0.5735	---
975	0.7080	0.7432	0.5761	---
1000	0.7115	0.7474	0.5788	1.0638
1005	0.7121	0.7482	0.5793	1.0651
1010	0.7128	0.7491	0.5798	1.0664
1015	0.7135	0.7499	0.5804	1.0677
1020	0.7142	0.7508	0.5809	1.0690
1025	0.7149	0.7516	0.5814	1.0703
1030	0.7156	0.7525	0.5819	1.0716
1035	0.7163	0.7533	0.5825	1.0729
1040	0.7170	0.7542	0.5830	1.0742
1041	0.7171	0.7544	0.5831	1.0745
1042	0.7173	0.7545	0.5832	1.0747
1043	0.7174	0.7547	0.5833	1.0750
1043.2	0.7174	0.7547	0.5834	1.0751
1044	0.7176	0.7549	0.5834	1.0753
1045	0.7177	0.7550	0.5835	1.0755
1050	0.7184	0.7559	0.5841	1.0769
1060	0.7198	0.7576	0.5852	1.0795
1070	0.7212	0.7594	0.5862	1.0822
1080	0.7226	0.7611	0.5873	1.0848
1090	0.7240	0.7628	0.5884	1.0875
1100	0.7255	0.7646	0.5895	1.0902
1150	0.7327	0.7735	0.5950	1.1039
1184	0.7376	0.7797	0.5988	1.1134
1200	0.7400	0.7826	0.6006	1.1180
1300	0.7552	0.8015	0.6122	1.1472
1400	0.7710	0.8214	0.6243	1.1779
1500	0.7874	0.8422	0.6368	1.2104
1600	0.8046	0.8641	0.6498	1.2447
1665	0.8162	0.8790	0.6585	1.2681
1700	0.8226	0.8872	0.6634	1.2810
1800	0.8413	0.9116	0.6775	1.3195
1809	0.8431	0.9138	0.6788	1.3231
1900	0.8610	0.9373	0.6923	1.3604
2000	0.8816	0.9645	0.7077	1.4039
2200	0.9258	1.0240	0.7407	1.4998
2400	0.9748	1.0914	0.7769	1.6098
2600	1.0292	1.1682	0.8169	1.7371
2800	1.0901	1.2566	0.8612	1.8864
3000	1.1586	1.3596	0.9105	2.0637

Table 12. Isothermal bulk modulus of the iron polymorphs as a function of the absolute temperature.

Temperature (K)	Fe(bcc)	Fe(fcc)	Fe(hcp)	Fe(liq)
	Mbar			
200	1.6225	1.5790	1.9796	---
225	1.6158	1.5714	1.9718	---
250	1.6090	1.5639	1.9639	---
273.15	1.6027	1.5569	1.9566	---
298.15	1.5959	1.5494	1.9487	---
300	1.5954	1.5489	1.9482	---
350	1.5819	1.5338	1.9324	---
400	1.5683	1.5187	1.9167	---
450	1.5547	1.5037	1.9009	---
500	1.5412	1.4886	1.8852	---
550	1.5276	1.4735	1.8695	---
600	1.5141	1.4585	1.8537	---
650	1.5005	1.4434	1.8380	---
700	1.4869	1.4284	1.8223	---
750	1.4734	1.4133	1.8065	---
800	1.4598	1.3982	1.7908	---
850	1.4463	1.3832	1.7750	---
900	1.4327	1.3681	1.7593	---
950	1.4191	1.3531	1.7436	---
975	1.4123	1.3455	1.7357	---
1000	1.4056	1.3380	1.7278	0.9400
1005	1.4042	1.3365	1.7262	0.9389
1010	1.4029	1.3350	1.7247	0.9377
1015	1.4015	1.3335	1.7231	0.9366
1020	1.4001	1.3320	1.7215	0.9355
1025	1.3988	1.3305	1.7200	0.9343
1030	1.3974	1.3290	1.7184	0.9332
1035	1.3961	1.3275	1.7168	0.9321
1040	1.3947	1.3259	1.7152	0.9309
1041	1.3944	1.3256	1.7149	0.9307
1042	1.3942	1.3253	1.7146	0.9305
1043	1.3939	1.3250	1.7143	0.9302
1043.2	1.3939	1.3250	1.7142	0.9302
1044	1.3936	1.3247	1.7140	0.9300
1045	1.3934	1.3244	1.7137	0.9298
1050	1.3920	1.3229	1.7121	0.9286
1060	1.3893	1.3199	1.7089	0.9264
1070	1.3866	1.3169	1.7058	0.9241
1080	1.3839	1.3139	1.7026	0.9218
1090	1.3812	1.3109	1.6995	0.9195
1100	1.3784	1.3079	1.6963	0.9172
1150	1.3649	1.2928	1.6806	0.9059
1184	1.3557	1.2826	1.6699	0.8981
1200	1.3513	1.2777	1.6649	0.8945
1300	1.3242	1.2476	1.6334	0.8717
1400	1.2971	1.2175	1.6019	0.8489
1500	1.2700	1.1874	1.5704	0.8262
1600	1.2428	1.1573	1.5390	0.8034
1665	1.2252	1.1377	1.5185	0.7886
1700	1.2157	1.1271	1.5075	0.7806
1800	1.1886	1.0970	1.4760	0.7578
1809	1.1861	1.0943	1.4732	0.7558
1900	1.1615	1.0669	1.4445	0.7351
2000	1.1343	1.0368	1.4131	0.7123
2200	1.0801	0.9765	1.3501	0.6667
2400	1.0259	0.9163	1.2871	0.6212
2600	0.9716	0.8560	1.2242	0.5757
2800	0.9174	0.7958	1.1612	0.5301
3000	0.8631	0.7355	1.0983	0.4846

Table 13. Isentropic compressibility of the iron polymorphs as a function of the absolute temperature.

Temperature (K)	Fe(bcc)	Fe(fcc)	Fe(hcp)	Fe(liq)
	Mbar^{-1}			
200	0.6104	0.6057	0.4839	---
225	0.6120	0.6069	0.4842	---
250	0.6136	0.6079	0.4845	---
273.15	0.6149	0.6087	0.4847	---
298.15	0.6163	0.6094	0.4849	---
300	0.6164	0.6095	0.4849	---
350	0.6190	0.6108	0.4852	---
400	0.6215	0.6119	0.4855	---
450	0.6240	0.6131	0.4857	---
500	0.6265	0.6144	0.4859	---
550	0.6293	0.6158	0.4860	---
600	0.6323	0.6175	0.4863	---
650	0.6357	0.6193	0.4865	---
700	0.6396	0.6213	0.4868	---
750	0.6440	0.6236	0.4872	---
800	0.6492	0.6261	0.4877	---
850	0.6554	0.6288	0.4883	---
900	0.6627	0.6318	0.4889	---
950	0.6719	0.6351	0.4897	---
975	0.6776	0.6368	0.4902	---
1000	0.6845	0.6386	0.4906	0.8901
1005	0.6862	0.6390	0.4907	0.8902
1010	0.6879	0.6393	0.4908	0.8902
1015	0.6898	0.6397	0.4909	0.8903
1020	0.6917	0.6401	0.4910	0.8903
1025	0.6939	0.6405	0.4911	0.8904
1030	0.6962	0.6408	0.4912	0.8904
1035	0.6988	0.6412	0.4913	0.8905
1040	0.7015	0.6416	0.4914	0.8905
1041	0.7021	0.6417	0.4915	0.8905
1042	0.7027	0.6418	0.4915	0.8905
1043	0.7033	0.6418	0.4915	0.8905
1043.2	0.7034	0.6419	0.4915	0.8905
1044	0.6797	0.6419	0.4915	0.8905
1045	0.6789	0.6420	0.4915	0.8905
1050	0.6755	0.6424	0.4917	0.8906
1060	0.6709	0.6432	0.4919	0.8906
1070	0.6681	0.6440	0.4921	0.8907
1080	0.6663	0.6448	0.4923	0.8907
1090	0.6649	0.6456	0.4926	0.8907
1100	0.6639	0.6464	0.4928	0.8908
1150	0.6616	0.6508	0.4941	0.8907
1184	0.6613	0.6539	0.4951	0.8906
1200	0.6614	0.6554	0.4955	0.8904
1300	0.6638	0.6654	0.4989	0.8891
1400	0.6684	0.6766	0.5028	0.8868
1500	0.6747	0.6890	0.5074	0.8834
1600	0.6825	0.7026	0.5127	0.8790
1665	0.6883	0.7122	0.5166	0.8755
1700	0.6917	0.7176	0.5187	0.8735
1800	0.7021	0.7341	0.5255	0.8669
1809	0.7031	0.7356	0.5262	0.8663
1900	0.7138	0.7520	0.5331	0.8593
2000	0.7268	0.7715	0.5415	0.8507
2200	0.7569	0.8160	0.5609	0.8307
2400	0.7927	0.8686	0.5841	0.8075
2600	0.8348	0.9310	0.6116	0.7826
2800	0.8840	1.0053	0.6439	0.7581
3000	0.9415	1.0942	0.6816	0.7378

Table 14. Isentropic bulk modulus of the iron polymorphs as a function of the absolute temperature.

Temperature	Fe(bcc)	Fe(fcc)	Fe(hcp)	Fe(liq)
(K)	Mbar			
200	1.6381	1.6510	2.0665	---
225	1.6339	1.6478	2.0652	---
250	1.6298	1.6451	2.0641	---
273.15	1.6263	1.6430	2.0631	---
298.15	1.6226	1.6409	2.0623	---
300	1.6224	1.6408	2.0622	---
350	1.6155	1.6373	2.0609	---
400	1.6091	1.6341	2.0598	---
450	1.6027	1.6310	2.0590	---
500	1.5961	1.6276	2.0582	---
550	1.5892	1.6238	2.0574	---
600	1.5816	1.6196	2.0565	---
650	1.5731	1.6148	2.0554	---
700	1.5636	1.6095	2.0541	---
750	1.5527	1.6037	2.0524	---
800	1.5402	1.5973	2.0504	---
850	1.5258	1.5903	2.0480	---
900	1.5089	1.5827	2.0452	---
950	1.4883	1.5746	2.0419	---
975	1.4758	1.5703	2.0401	---
1000	1.4608	1.5659	2.0382	1.1234
1005	1.4574	1.5650	2.0378	1.1234
1010	1.4537	1.5641	2.0374	1.1233
1015	1.4498	1.5632	2.0370	1.1232
1020	1.4456	1.5623	2.0366	1.1232
1025	1.4412	1.5614	2.0361	1.1231
1030	1.4363	1.5605	2.0357	1.1231
1035	1.4311	1.5595	2.0353	1.1230
1040	1.4255	1.5586	2.0348	1.1230
1041	1.4243	1.5584	2.0347	1.1230
1042	1.4231	1.5582	2.0347	1.1229
1043	1.4219	1.5580	2.0346	1.1229
1043.2	1.4217	1.5580	2.0345	1.1229
1044	1.4712	1.5578	2.0345	1.1229
1045	1.4730	1.5576	2.0344	1.1229
1050	1.4804	1.5567	2.0339	1.1229
1060	1.4905	1.5548	2.0330	1.1228
1070	1.4967	1.5529	2.0321	1.1227
1080	1.5009	1.5509	2.0311	1.1227
1090	1.5039	1.5489	2.0302	1.1227
1100	1.5062	1.5469	2.0292	1.1226
1150	1.5114	1.5367	2.0238	1.1227
1184	1.5121	1.5294	2.0199	1.1229
1200	1.5120	1.5259	2.0180	1.1230
1300	1.5066	1.5029	2.0045	1.1247
1400	1.4961	1.4780	1.9888	1.1277
1500	1.4821	1.4514	1.9707	1.1320
1600	1.4652	1.4232	1.9504	1.1377
1665	1.4528	1.4040	1.9359	1.1421
1700	1.4458	1.3934	1.9277	1.1448
1800	1.4243	1.3623	1.9029	1.1535
1809	1.4223	1.3594	1.9005	1.1543
1900	1.4009	1.3298	1.8759	1.1637
2000	1.3758	1.2961	1.8468	1.1755
2200	1.3211	1.2255	1.7829	1.2038
2400	1.2615	1.1513	1.7120	1.2384
2600	1.1979	1.0741	1.6351	1.2778
2800	1.1312	0.9948	1.5531	1.3191
3000	1.0622	0.9139	1.4671	1.3553