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High-Temperature Relative Enthalpies and Related Thermodynamic Properties of CuI

By M. J. Ferrante, R. V. Mrazek, and R. R. Brown



UNITED STATES DEPARTMENT OF THE INTERIOR

Report of Investigations 9074

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Donald Paul Hodel, Secretary

BUREAU OF MINES
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Library of Congress Cataloging in Publication Data:

Ferrante, M. J. (Michael John), 1930-

High-temperature relative enthalpies and related thermodynamic properties of CuI.

(Report of investigations ; 9074)

Bibliography: p. 9-10.

Supt. of Docs. no.: I 28.23: 9074.

1. Cuprous iodide--Thermal properties. 2. High temperatures. I. Mrazek, R. V. (Robert V.). II. Brown, R. R. (Robert R.). III. Title. IV. Series: Report of investigations (United States. Bureau of Mines) ; 9074.

TN23.U43

[QD181.I1]

622 s [546'.6522]

86-607924

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UNIT OF MEASURE ABBREVIATIONS USED IN THIS REPORT

| | | | |
|-------------------|--------------------------------|----------|----------------------|
| cal | calorie | K | kelvin |
| cal/(mol·K) | calorie per mole per kelvin | kcal/mol | kilocalorie per mole |
| cm ³ | cubic centimeter | min | minute |
| deg | degree | mL | milliliter |
| g | gram | μK | microkelvin |
| g/cm ³ | gram per cubic centimeter | μV | microvolt |
| h | hour | pct | percent |
| J | joule | wt pct | weight percent |

HIGH-TEMPERATURE RELATIVE ENTHALPIES AND RELATED THERMODYNAMIC PROPERTIES OF CuI

By M. J. Ferrante,¹ R. V. Mrazek,² and R. R. Brown¹

ABSTRACT

Relative enthalpies of cuprous iodide (CuI) were measured at the Bureau of Mines to provide thermodynamic data for the advancement of mineral technology. Enthalpy measurements between 298.15 and 1,396.3 K were made with a copper-block drop calorimeter. The temperatures of transition were measured by differential scanning calorimetry (DSC). Reversible transitions were determined at 643 K with a standard enthalpy of transition (ΔH_{tr}°) = 0.74 kcal/mol, at 679 K with a ΔH_{tr}° = 0.65 kcal/mol, and at 868 K with a standard enthalpy of fusion (ΔH_m°) = 1.895 kcal/mol. Tabulated values are listed at selected temperature increments from 298.15 to 1,600 K for the standard relative enthalpy ($H^{\circ} - H_{298}^{\circ}$), heat capacity (C_p°), entropy (S°), and Gibbs energy function [$-(G^{\circ} - H_{298}^{\circ})/T$]. The enthalpy data are also given in the form of equations and combined with thermodynamic data from other investigations to derive values of standard enthalpies of formation (ΔH_f°), Gibbs energies of formation (ΔG_f°), and logarithms of the equilibrium constants of formation ($\log K_f$).

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INTRODUCTION

The relative enthalpies of cuprous iodide (CuI) were measured by the Bureau of Mines to provide reliable thermodynamic data for the correction of some of the problems of copper technology described by Schroeder (1).³ The present investigation is part of a program by the Bureau to determine the thermodynamic properties of important copper compounds such as those reported by Ferrante (2-3) and Beyer (4). In addition, a monograph on the thermodynamic properties of copper and its inorganic compounds was compiled by King (5).

No reliable high-temperature thermodynamic data for CuI could be found in the literature. Experimental measurements of heat capacities or relative enthalpies above 298.15 K reported by Carré (6), Miyake (7), and Nölting (8) could not be adequately interpreted because the data were only shown graphically. The enthalpy data given by Carré were also badly scattered. Le-Van-My (9) and Ghosh (10) listed only the temperature and enthalpy of transition for the

phase changes. None of these investigators presented standard enthalpies of formation or Gibbs energies of formation. Complete thermodynamic data are reported in the present investigation, and these reliable results consist of relative enthalpies measured with a copper-block calorimeter and transition temperatures determined with a differential scanning calorimeter-thermogravimetric analyzer (DSC-TGA). The DSC investigation was also made to clarify the anomalous rise in heat capacity before the first crystal transition.

Unless designated otherwise, CuI refers to the stable α -phase that exists from 0 to 643 K and has a face-centered cubic structure as shown on the Powder Diffraction File (PDF) card 6-246. The β -phase exists between 643 and 679 K and has a hexagonal structure as listed on PDF card 6-685. The γ -phase exists from 679 K to the melting point at 868 K and crystallizes in a body-centered cubic structure as given on PDF card 6-623.

MATERIALS

The CuI used was ultrapure material. The material was purchased from Alpha⁴ and purified in 50-g lots as follows: Each lot was digested with 100 mL water and 5 mL HI (hydroiodic acid) by heating to boiling and maintaining boiling for about 15 min. After cooling, the liquid was decanted off, fresh liquid was added, and the procedure was repeated a total of five times. The final solution was removed by suction filtering, and the solid was washed first with 100 mL of methanol containing 0.5 mL HI, and then with anhydrous methanol. The CuI was then

dried under vacuum for 2 days. All of the lots were blended together before preparing samples for analyses and the determination of thermodynamic properties.

Chemical analyses of the dried material showed 33.38 pct Cu and 66.60 pct I, compared with theoretical values of 33.37 pct and 66.63 pct, respectively. Optical emission spectroscopy detected only silicon at less than 0.01 pct. X-ray powder diffraction analysis showed that the pattern matched PDF card 6-246 for the room-temperature α -phase of CuI.

EXPERIMENTAL WORK AND RESULTS

Enthalpies relative to 298.15 K were measured with a drop calorimeter in an isothermal jacket. In this method, an

encapsulated sample was heated in a furnace to a known temperature and dropped into the copper block. In order

³Underlined numbers in parentheses refer to items in the list of references at the end of this report.

⁴Reference to specific products does not imply endorsement by the Bureau of Mines.

to provide a nearly isothermal region for heating the sample, one furnace with a cylindrical heat sink of silver was used to 1,200 K, and another furnace with a cylindrical heat sink of platinum was used between 1,200 and 1,400 K. The temperature of the sample in both furnaces was measured with platinum versus platinum-10 wt pct rhodium thermocouples, which were calibrated against the melting point of gold as required according to previously established temperature-time criteria. The temperature of the calorimeter was measured with a transposed-bridge-type resistance thermometer that is wound around the copper block, which provides a significantly greater temperature sensitivity than a single winding. The use of the resistance thermometer in conjunction with a six-dial potentiometer and nanovolt null detector can resolve changes equivalent to $\pm 50 \mu\text{K}$ or $\pm 0.02 \mu\text{V}$. Before and after a series of enthalpy determinations for each substance, the calorimeter was calibrated electrically, and the constancy of this calibration served as a check on the precision of measurements. The average deviation of the electrical calibrations was 0.02 pct. The enthalpy of periclase (MgO) was also measured before and after a series of enthalpy determinations for each substance to serve as an overall check of the entire equipment. Results of the MgO measurements agreed within 0.1 pct with the values derived by Pankratz (11) from studies conducted by Barron (12), Victor (13), and Pankratz (14). Detailed descriptions of the construction and operation of the drop calorimeter and furnaces are given by Ferrante (15).

Experimental measurements of relative enthalpies were made with CuI sealed in a capsule of pure silica (SiO_2). After the capsule was filled with powdered CuI in air, it was evacuated overnight. The neck of the evacuated capsule was sealed by fusion while the portion of the capsule containing the CuI was immersed in ice water. The CuI in the sealed capsule was melted by heating at 1,510 K for 1 h, and the melt was quenched on an aluminum block. Under these conditions, X-ray powder diffraction of the capsule contents disclosed only the room-temperature

α -phase, thus showing the reversibility of the phase transitions. Enthalpy measurements were then made with another sample of CuI sealed in a SiO_2 capsule, melted at 990 K, and quenched as just described. For this sample, a mass of 11.74729 g CuI was sealed in 5.23726 g SiO_2 . This amount of SiO_2 contributed an average of 52 pct of the total enthalpy measured for the CuI sample and the SiO_2 capsule. The enthalpy change of the empty SiO_2 capsule was measured in separate experiments. The empty capsule had an internal volume of 4.21 cm^3 . The volume of CuI in the capsule was calculated to be 2.06 cm^3 , based upon a density of 5.71 g/cm^3 . The mass of the filled capsule was periodically checked for constancy by weighing between enthalpy measurements. The molecular weight of 190.451 for CuI conforms to the 1981 Table of Atomic Weights (16).

The relative enthalpies are expressed in terms of the thermochemical calorie where $1 \text{ cal} = 4.1840 \text{ J}$. Enthalpy measurements were conducted after the sample attained the desired temperature, which was then maintained an additional 1.5 to 2 h. Measurements made with double these residence times showed no change in relative enthalpy. Therefore, the sample and capsule attained temperature equilibrium in the furnace at the minimum residence time, which was employed in 85 pct of the measurements. The results of experimental measurements were converted to kilocalories per mole and are listed in table 1 in order of increasing temperatures as standard enthalpies relative to 298.15 K ($H^\circ - H_{298}^\circ$). The temperature (T) is in kelvin as defined by the International Temperature Scale of 1968 (17). The data in table 1 also show the reversibility of phase transitions when the runs are arranged sequentially, as discussed later. In addition, the percent deviation between the experimental and smoothed values is given. Smoothed values are given in the "Discussion" section.

The transition temperatures for CuI were also measured with a DSC-TGA, Mettler model TA2000C. The instrument was calibrated at the melting points of indium (429.75 K) and of gold (1,337.58 K). Both of these standards were better than

TABLE 1. - Experimental relative enthalpies of CuI(c,l)

| T, K | H° - H ₂₉₈ ^o , kcal/mol | Deviation, ¹ pct | Run | T, K | H° - H ₂₉₈ ^o , kcal/mol | Deviation, ¹ pct | Run |
|--------------------|--|--------------------------------|-----|----------------------|--|--------------------------------|-----|
| ² 402.6 | 1.389 | -0.12 | 1 | 752.3 | 9.134 | 0.26 | 8 |
| 443.3 | 1.948 | -.03 | 2 | 802.1 | 9.940 | .13 | 16 |
| 502.6 | 2.787 | .12 | 3 | 851.0 | 10.715 | -.13 | 17 |
| 555.1 | 3.568 | -.15 | 4 | 865.0 | 10.960 | .02 | 18 |
| 601.2 | 4.349 | .16 | 9 | 870.4 | 12.933 | -.06 | 24 |
| 621.7 | 4.757 | -.05 | 10 | 880.1 | 13.091 | -.03 | 23 |
| 627.3 | 4.889 | -.05 | 5 | 901.8 | 13.449 | .09 | 19 |
| 640.3 | 5.236 | -.13 | 12 | 1,001.3 | 14.978 | .04 | 20 |
| 645.9 | 6.171 | .14 | 13 | 1,103.8 | 16.505 | .03 | 21 |
| 651.9 | 6.356 | -.07 | 6 | ³ 1,111.2 | 16.587 | -.13 | 25 |
| 665.5 | 6.800 | -.16 | 14 | 1,194.3 | 17.835 | .15 | 22 |
| 677.9 | 7.231 | .13 | 11 | ³ 1,209.1 | 18.001 | -.11 | 26 |
| 686.3 | 8.004 | -.29 | 15 | ³ 1,301.9 | 19.323 | -.01 | 27 |
| 702.1 | 8.294 | .09 | 7 | ³ 1,396.3 | 20.627 | .01 | 28 |

¹Deviation between experimental and smoothed values.

²CuI melted at 990 K for 1 h before starting measurements.

³Furnace with Pt heat sink used; other measurements used furnace with silver heat sink.

99.99 pct pure. This temperature calibration showed an accuracy of ± 0.3 K for temperature measurements. The temperature calibration was confirmed by measuring the temperature of solid-solid and solid-liquid transitions of selected compounds and metals. Results of these measurements are listed in table 2 and

are in good agreement with the values reported by Breuer (18), Rajeshwar (19), and Pankratz (11). Data by Breuer and Rajeshwar were obtained by DSC measurements using Du Pont thermal analyzers 1090 and 990, respectively. Table 2 also shows the measured transition temperatures for CuI.

DISCUSSION

Relative enthalpy measurements were smoothed using a curve-fitting program developed by Justice (20). In this process, the high-temperature data were smoothly merged with the low-temperature data reported by King (5). The fitting process used polynomials to derive the smooth thermodynamic values shown in table 3 at selected temperature intervals. The tabulated values are listed to three decimals to maintain internal consistency among the values, even though the experimental precision does not warrant this exactness. The smooth enthalpies of table 3 are estimated to have an absolute uncertainty of ± 0.3 pct. The standard deviation of the experimental enthalpies from the smooth values was 0.13 pct. Polynomials from the computer program were also used to derive smooth values of relative enthalpies at the

temperatures of the experimental measurements in order to calculate the deviations shown in table 1. The average deviation of the measurements was 0.10 pct.

The DSC is a more precise technique for measuring temperatures of transition than drop calorimetry; however, the DSC is not as precise for determining enthalpies of transition, except for slow solid-solid transitions. Thus, the transition temperatures were established by the DSC, and enthalpies of transition by the drop calorimeter. Three reversible transitions were shown by the thermal behavior of CuI. Temperatures of transition were measured by the DSC at 642.8 ± 0.3 , 679.1 ± 0.3 , and 868.4 ± 0.3 K. These temperatures were rounded to the nearest degree for the derivation of thermodynamic quantities from enthalpy measurements.

TABLE 2. - Transition temperatures measured by DSC

| Substance | Transition ¹ | T, K | | Substance | Transition ¹ | T, K | |
|------------------------|-------------------------|-------------------------|--------------------|--------------------------------------|-------------------------|-------------------------|--------------------|
| | | Literature ² | This investigation | | | Literature ² | This investigation |
| In..... | MP | 430.15 | 429.8 | Zn..... | MP | 692.15 | 692.7 |
| Sn..... | MP | 505.15 | 505.1 | Ag ₂ SO ₄ | ss | 699.15 | 700.1 |
| KClO ₄ | ss | 573.15 (19) | 572.6 | CsCl..... | ss | 749.15 | 740.2 |
| Cd..... | MP | 594.15 | 594.0 | CuI(γ-ℓ).. | MP | ³ 873- | 868.4 |
| CuI(α-β).. | ss | ³ 642- | 642.8 | | | 875 | |
| | | 653 | | Al..... | MP | 933.61 (11) | 934.3 |
| CuI(β-γ).. | ss | ³ 670- | 679.1 | K ₂ CrO ₄ | ss | 941.15 | 943.6 |
| | | 693 | | | | | |

¹MP = melting point; ss = solid-solid transition.

²All data by Breuer (18) unless otherwise noted by a reference number.

³See "Discussion" section.

TABLE 3. - High-temperature thermodynamic properties of CuI(c,ℓ)

| T, K | cal/(mol·K) | | | H° - H ₂₉₈ ^o , kcal/mol |
|------------------|-----------------------------|----------|--|--|
| | C _p ^o | S° | -(G° - H ₂₉₈ ^o)/T | |
| 298.15 | 12.920 | 23.087 | 23.087 | 0 |
| 300 | 12.940 | 23.167 | 23.087 | .024 |
| 350 | 13.348 | 25.180 | 23.245 | .677 |
| 400 | 13.672 | 26.989 | 23.601 | 1.355 |
| 450 | 13.812 | 28.604 | 24.069 | 2.041 |
| 500 | 14.481 | 30.088 | 24.597 | 2.746 |
| 550 | 15.481 | 31.513 | 25.160 | 3.494 |
| 600 | 18.380 | 32.947 | 25.748 | 4.320 |
| ¹ 643 | 31.534 | 34.561 | 26.278 | 5.326 |
| 643 | 33.100 | 35.712 | 26.278 | 6.066 |
| 650 | 33.100 | 36.070 | 26.382 | 6.298 |
| ² 679 | 33.100 | 37.515 | 26.826 | 7.258 |
| 679 | 16.400 | 38.472 | 26.826 | 7.908 |
| 700 | 16.400 | 38.971 | 27.183 | 8.252 |
| 750 | 16.400 | 40.103 | 28.007 | 9.072 |
| 800 | 16.400 | 41.161 | 28.797 | 9.892 |
| 850 | 16.400 | 42.155 | 29.554 | 10.712 |
| ³ 868 | 16.400 | 42.499 | 29.818 | 11.007 |
| 868 | 15.903 | 44.682 | 29.818 | 12.902 |
| 900 | 15.714 | 45.256 | 30.357 | 13.408 |
| 950 | 15.431 | 46.098 | 31.164 | 14.187 |
| 1,000 | 15.165 | 46.882 | 31.930 | 14.952 |
| 1,050 | 14.915 | 47.616 | 32.660 | 15.704 |
| 1,100 | 14.681 | 48.305 | 33.356 | 16.444 |
| 1,150 | 14.464 | 48.952 | 34.020 | 17.172 |
| 1,200 | 14.263 | 49.564 | 34.655 | 17.890 |
| 1,250 | 14.078 | 50.142 | 35.263 | 18.599 |
| 1,300 | 13.910 | 50.691 | 35.846 | 19.298 |
| 1,350 | 13.757 | 51.213 | 36.405 | 19.990 |
| 1,400 | 13.621 | 51.711 | 36.943 | 20.674 |
| 1,450 | (13.502) | (52.187) | (37.461) | (21.352) |
| 1,500 | (13.398) | (52.642) | (37.959) | (22.025) |
| 1,550 | (13.311) | (53.080) | (38.440) | (22.693) |
| 1,600 | (13.241) | (53.502) | (38.904) | (23.356) |

¹α-β transition. ²β-γ transition. ³Melting point.

NOTE.--Values in parentheses are extrapolations.

Accordingly, the transitions at 643, 679, and 868 K are illustrated graphically in figure 1, which depicts the relationship between the smoothed and experimental enthalpies as the mean heat capacity, $(H^\circ - H_{298}^\circ)/(T-298.15)$, versus T. The reversibility of the phase transitions and the reproducibility of the enthalpy measurements were verified when measurements made at temperatures above and then below the transitions again fell on the smooth curve of the mean heat capacity. (See sequential order of runs in table 1 and then figure 1.)

The first solid-solid transition was found between 640.3 and 645.9 K by relative enthalpy measurements. The selected temperature for this transition was established at 643 K after rounding the temperature measured by the DSC at 642.8 ± 0.3 K. Enthalpy data at 643 K gave a standard enthalpy of transition (ΔH_{tr}°) of 0.74 kcal/mol. An anomalous increase in heat capacity starting about 150 deg below the transition temperature of 643 K was found; however, the bulk of the heat absorption occurred isothermally at the transition temperature. This anomaly for the crystal transition was also found by the DSC of this investigation and by heat-capacity measurements made with the adiabatic calorimeter of Nölting (8) and Miyake (7). Nölting gave a transition temperature of 642 K. Miyake reported a transition temperature of 642 K with an estimated ΔH_{tr}° of 1.7 kcal/mol. Both Miyake and Nölting showed their experimental measurements of heat capacity only graphically, and their data could not be satisfactorily evaluated. Le-Van-My (9) reported a ΔH_{tr}° of 0.61 kcal/mol at 648 K by averaging measurements made by differential thermal analysis (DTA). Similar work by Ghosh (10) gave average values of 1.18 kcal/mol and 643.9 K. Carré (6) measured transition temperatures with a DTA and relative enthalpies with a copper-block calorimeter; however, his experimental enthalpies were badly scattered and were only depicted graphically. He gave a temperature of 653 K with $\Delta H_{tr}^\circ = 1.95$ kcal/mol. His enthalpy data for each of the CuI phases were represented by equations. Enthalpy values calculated from the equation representing the data

given by Carré from 486 to 653 K were from 21 pct to 29 pct above the data of the present investigation.

Experimental enthalpy measurements showed that the second crystal transition of CuI was between 677.9 and 686.3 K, and the selected transition temperature of 679 was established from rounding the DSC measurement at 679.1 ± 0.3 K. Enthalpy data at the rounded temperature gave $\Delta H_{tr}^\circ = 0.65$ kcal/mol. Temperatures and/or enthalpies of transition reported by other investigators were 681 K by Nölting, 685 K and 0.66 kcal/mol by Le-Van-My, 680 K and an estimated 0.77 kcal/mol by Miyake, 693 K and 0.63 kcal/mol by Carré, and 670 K with an estimated 0.19 kcal/mol by Ghosh. The relative enthalpies calculated from the equation representing the data of Carré from 653 to 693 K were 24 pct higher than the values of the present investigation.

The measurements for the third transition of CuI from the solid to liquid phase established a melting point at 868 K from the DSC and a standard enthalpy of fusion (ΔH_m°) of 1.895 kcal/mol from the drop calorimeter. A fusion temperature of 868.4 ± 0.3 K was actually measured by the DSC. The fusion temperature from the DSC was verified by drop calorimeter measurements that showed the temperature was between 865.0 and 870.4 K. Nölting gave a melting temperature of 875 K, and Le-Van-My gave a melting point of 873 K with $\Delta H_m^\circ = 0.95$ kcal/mol. Carré listed 873 K with $\Delta H_m^\circ = 1.975$ kcal/mol. The equation representing the data of Carré for the liquid phase gave relative enthalpies from 11 pct to 14 pct above those of the present investigation, while his equation for γ -CuI gave values that were from 11 to 15 pct above those of this work.

Enthalpy measurements were discontinued at about 1,400 K to prevent devitrification of the SiO₂ capsule. X-ray powder diffraction analysis of the CuI removed from the capsule after completion of relative enthalpy measurements yielded the same pattern as that of the starting material, α -phase CuI. No vapor pressure correction was necessary even at the highest extrapolated temperature of 1,600 K because the data of Krabbes (21)

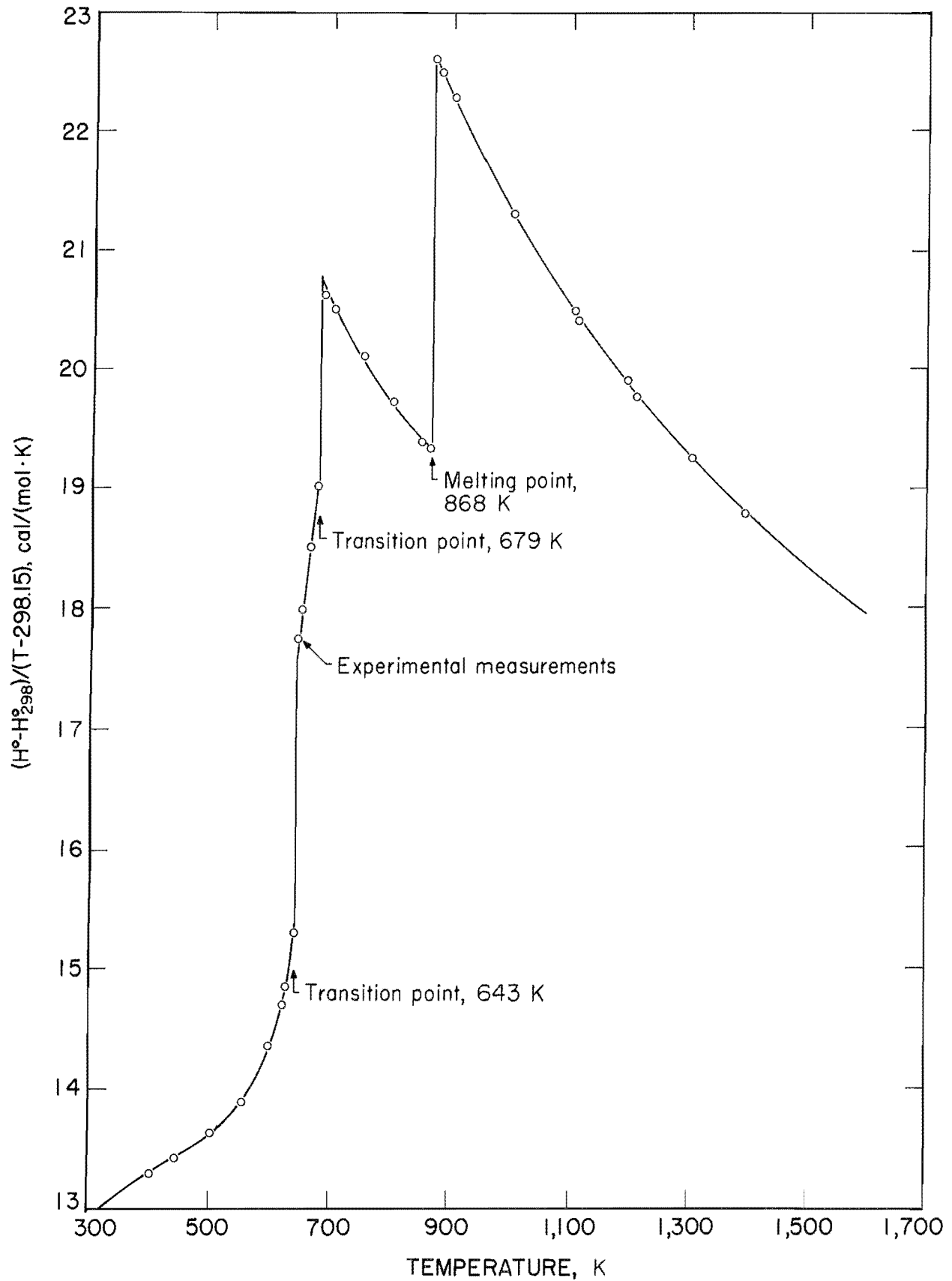


FIGURE 1.—Variation of mean heat capacity with temperature for $\text{CuI}(\text{c}, \ell)$.

showed the correction would be less than 0.03 pct.

The smoothed enthalpies presented in tabular form (table 3) are now given in simplified algebraic forms to better meet the needs of various users. The equations were derived from the smooth enthalpies of table 3 by Kelley's method (22). Because these equations contain six or fewer digits in a maximum of four terms, they give less precise enthalpies than the tabulated values calculated from the polynomials. However, the polynomials are not given because they can have up to 10 terms, with each term having 17 digits, and rounding of these numbers results in significant differences from the precise smooth values given in tabular form. The simplified equations derived by Kelley's method are obviously more convenient to use than the polynomials. The equations have been widely adopted as the standard form for the algebraic representation of high-temperature enthalpies because they give an adequate fit of the values without introducing undue complexity. The equations are expressed in kilocalories per mole and are given below with the temperature range of validity and the average deviation from the smoothed data shown in parentheses after each equation:

$$\begin{aligned} \alpha: \quad H^\circ - H_{298.15}^\circ &= -8.478 \times 10^{-3}T \\ &+ 21.064 \times 10^{-6}T^2 \\ &- 7.855 \times 10^2 T^{-1} \\ &+ 3.290 \end{aligned}$$

(298-643 K; 2.1 pct)

$$\Delta H_{643}^\circ(\alpha-\beta) = 0.74.$$

$$\begin{aligned} \beta: \quad H^\circ - H_{298.15}^\circ &= 33.100 \times 10^{-3}T \\ &- 15.217 \end{aligned}$$

(643-679 K; <0.01 pct)

$$\Delta H_{679}^\circ(\beta-\gamma) = 0.65.$$

$$\begin{aligned} \gamma: \quad H^\circ - H_{298.15}^\circ &= 16.400 \times 10^{-3}T \\ &- 3.228 \end{aligned}$$

(679-868 K; <0.01 pct)

$$\Delta H_{868}^\circ = 1.895.$$

$$\begin{aligned} \ell: \quad H^\circ - H_{298.15}^\circ &= 16.693 \times 10^{-3}T \\ &- 1.321 \times 10^{-6}T^2 \\ &- 11.321 \times 10^2 T^{-1} \\ &+ 0.712 \end{aligned}$$

(868-1,600 K; 0.03 pct).

The average deviation of 2.1 pct for the equation of the α -phase is much higher than usual because of the anomalous increase in heat capacity before this transition. The average deviation of less than 0.01 pct for the β - and γ -phases shows that little accuracy is lost in using enthalpies calculated from the equations for the β - and γ -phases instead of the tabulated values. Even the equation for the ℓ -phase is a fairly good representation of the smoothed values because its average deviation is only 0.03 pct.

Standard enthalpies of formation (ΔH_f°), Gibbs energies of formation (ΔG_f°), and logarithms to the base 10 of the equilibrium constants of formation ($\log K_f$) were derived as functions of temperature for CuI by combining relative enthalpies from the present investigation with supplementary data from King (5). The results of these calculations are listed in table 4.

TABLE 4. - Formation data for $\text{Cu}(c,\ell) + 0.5 \text{I}_2(c,\ell,g) = \text{CuI}(c,\ell)$

| T, K | kcal/mol | | Log Kf | T, K | kcal/mol | | Log Kf |
|--------------------|--------------------|--------------------|--------|----------------------|--------------------|--------------------|--------|
| | ΔH_f° | ΔG_f° | | | ΔH_f° | ΔG_f° | |
| 298.15 | -16.200 | -16.583 | 12.155 | ⁵ 868 | -18.788 | -11.857 | 2.985 |
| 300 | -16.199 | -16.585 | 12.082 | 868 | -16.893 | -11.857 | 2.985 |
| ¹ 386.8 | -16.166 | -16.701 | 9.436 | 900 | -16.746 | -11.675 | 2.835 |
| 386.8 | -18.021 | -16.701 | 9.436 | 1,000 | -16.330 | -11.134 | 2.433 |
| 400 | -18.048 | -16.656 | 9.100 | 1,100 | -15.984 | -10.631 | 2.112 |
| ² 458.4 | -18.171 | -16.443 | 7.840 | 1,200 | -15.707 | -10.158 | 1.850 |
| 458.4 | -23.181 | -16.443 | 7.840 | 1,300 | -15.500 | -9.705 | 1.632 |
| 500 | -23.028 | -15.838 | 6.923 | ⁶ 1,357.6 | -15.416 | -9.453 | 1.522 |
| 600 | -22.529 | -14.440 | 5.260 | 1,357.6 | -18.536 | -9.453 | 1.522 |
| ³ 643 | -21.989 | -13.876 | 4.716 | 1,400 | -18.481 | -9.170 | 1.432 |
| 643 | -21.249 | -13.876 | 4.716 | 1,500 | -18.366 | -8.509 | 1.240 |
| ⁴ 679 | -20.449 | -13.485 | 4.340 | 1,600 | -18.272 | -7.854 | 1.073 |
| 679 | -19.799 | -13.485 | 4.340 | | | | |
| 700 | -19.685 | -13.291 | 4.150 | | | | |
| 800 | -19.147 | -12.414 | 3.391 | | | | |

¹Melting point of I_2 .³ α - β transition of CuI.⁵Melting point of CuI.²Boiling point of I_2 .⁴ β - γ transition of CuI.⁶Melting point of Cu.

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