

Thermodynamics of copper sulfides

II. Heat capacity and thermodynamic properties of synthetic covellite, CuS, from 5 to 780.5 K. Enthalpy of decomposition^a

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The heat capacity of CuS has been measured by adiabatic shield calorimetry from 5 to 840 K. The heat capacity increases regularly up to about 750 K and then more strongly as the decomposition temperature (780.5 K) of covellite into high-digenite and sulfur is approached. The molar enthalpy and molar entropy of decomposition are $2149.3R \cdot K$ and $2.755R$. Above 780.5 K the uptake of sulfur in the high-digenite causes a further rise in the heat capacity. The low-temperature values increase more strongly than expected from the Debye relation with a Debye temperature estimated from the intermediate-temperature behavior. This phenomenon as well as a small bump in the heat capacity around 55 K are discussed. The resulting molar enthalpy and molar entropy at 298.15 and 825 K are $1136.6R \cdot K$, $8.101R$, and $6744.2R \cdot K$, $17.393R$, respectively.

1. Introduction

In this series of papers on the thermodynamic properties of copper sulfides, the present one concerns the heat capacity of covellite, CuS, and the derived thermodynamic properties.

The crystal structure of covellite was solved by Oftedal⁽²⁾ in 1932. It is hexagonal (space group $P6_3/mmc$, $a = 380$ pm, $c = 1640$ pm) with 6 CuS formula units in the unit cell. Later refinements of the structure have mainly confirmed the results of Oftedal,^(3–7) but also led to more accurate structural parameters. Of the 6 Cu atoms 4 are tetrahedrally coordinated and 2 are triangularly coordinated by S atoms. Four of the 6 S atoms form S_2 groups. In accordance with this, the S (2p) X-ray photoelectron spectrum of CuS shows a doublet structure corresponding to the two

^a The preceding paper in this series is cited in reference 1.

different coordinations (octahedrally and triangularly bipyramidal) of S atoms.⁽⁸⁻⁹⁾ However, all S atoms are in the same oxidation state with an average oxidation number of -1 .⁽⁸⁻⁹⁾

The solid-solution field of covellite is very small. Kullerud⁽¹⁰⁾ showed that covellite is stoichiometric within ± 0.002 of the $n(\text{Cu})/n(\text{S})$ mole ratio. More recently, Potter⁽¹¹⁾ found that the width of the solid-solution field did not exceed ± 0.0005 . In the same study the upper stability limit of covellite was extrapolated to be (782 ± 8) K, in good agreement with the findings of Kullerud.⁽¹⁰⁾

A cubic form of CuS has been reported by Kazinets.⁽¹²⁾ The electron-diffraction results presented can, however, be readily interpreted as a mixture of hexagonal chalcocite and high digenite.⁽¹¹⁾ Okamoto *et al.*⁽¹³⁾ observed what they denoted as "indistinct polymorphic phase transitions" in the temperature region 90 to 310 K. Such transitions have not been confirmed by other investigators.

The low-temperature heat capacity of covellite has been reported in previous investigations.⁽¹⁴⁻¹⁷⁾ In the most recent, released during the course of this study, Ferrante *et al.*⁽¹⁷⁾ presented heat capacities from 5 to 310 K, and enthalpies from 298 to 750 K by drop calorimetry. In addition, the heat capacity was extrapolated to the decomposition temperature of covellite, 780 K.

In the present study the temperature range has been extended to include the decomposition of covellite into high-digenite and sulfur. The heat capacities are corrected for the enthalpy of vaporization of liquid sulfur. In the temperature range 680 to 800 K this correction is based on previous published decomposition pressures,⁽¹⁸⁻²¹⁾ whereas the correction at higher temperatures is based on new equilibrium pressures obtained by the dew-point method.

2. Experimental

The copper sulfide was prepared directly from the elements. The copper was in the form of a continuous rod, >99.999 mass per cent pure, from the American Smelting and Refining Co., New Jersey. The sulfur was 99.9999 mass per cent pure crystals from Koch-Light Laboratories Ltd., Colnbrook, England. The mixture of the elements was heated in an evacuated and sealed vitreous-silica tube, constricted at the middle by a smaller-diameter tube. Copper was placed in one part of the tube and sulfur in the other, and the tube was put into a slightly inclined tube furnace with the sulfur-containing compartment protruding. The copper was heated to 620 K and the sulfur was allowed to melt and flow into the hotter part of the tube. After most of the sulfur had combined with the copper, a heating pad wound around the exterior end of the silica tube was used to bring the remaining sulfur into reaction overnight. The empty half of the silica tube was sealed off and discarded before the sample was tempered at 670 K for 24 h. The sample was then finally crushed and transferred to the calorimetric ampoule.

The characterization of the samples was done by powder X-ray diffraction. Room-temperature photographs were taken in a Guinier camera of 80 mm diameter with Cu $K\alpha_1$ radiation and silicon as calibration substance, $a(293.15 \text{ K}) = 543.1065 \text{ pm}$.⁽²²⁾ Unit-cell dimensions were derived by the method of least

TABLE 1. Unit-cell dimensions for covellite

a/pm	c/pm	Authors	a/pm	c/pm	Authors
381.0 ± 0.8	1646	Roberts and Ksanda ⁽²⁴⁾	379.6 ± 0.4	1636.0 ± 1.5	Kalbskopf <i>et al.</i> ⁽⁵⁾
376	1626	Alsén ⁽²⁵⁾	379.38 ± 0.05	1634.1 ± 0.1	Evans and Konner ⁽⁶⁾
380	1640	Oftedal ⁽²⁾	379.38 ± 0.05	1634.1 ± 0.1	Potter and Evans ⁽²⁸⁾
379.6	1636	Berry ⁽³⁾	379.6 ± 0.1	1638.2 ± 0.5	Ohmasa <i>et al.</i> ⁽⁷⁾
379.2	1634.4	Swanson <i>et al.</i> ⁽²⁶⁾	379.4	1634	Satish <i>et al.</i> ⁽²⁹⁾
379.4 ± 0.3	1633.2 ± 1.0	Djurle ⁽²⁷⁾	379.2 ± 0.4	1634.2 ± 0.3	Present work
379.0 ± 0.1	1634.0 ± 0.4	Bernadini and Catani ⁽⁴⁾			

squares using the program CELLKANT.⁽²³⁾ The obtained unit-cell dimensions as well as those by previous investigators are given in table 1.

The calorimetry was the same as that previously described⁽¹⁾ except that helium was used at 2.15 kPa pressure in the calorimeter at the University of Michigan⁽³⁰⁾ and that measurements were made from 300 to 840 K in the calorimeter at the University of Oslo.⁽³¹⁾ The heat capacities of the empty calorimeters were determined in separate series of experiments. The heat capacity of the empty calorimeter represented from 5 to 21 per cent of the total in the low-temperature calorimeter and 50 to 52 per cent in the high-temperature calorimeter, outside the decomposition region.

Small corrections were applied for temperature excursions of the shields from the calorimeter temperature. Further corrections were applied for differences in amounts of (indium + tin) solder, helium gas, and Apiezon-T grease for the low-temperature calorimeter and for differences in mass of the silica-glass containers for the high-temperature calorimeter. The masses of CuS were 130.481 g and 132.276 g in the low- and high-temperature calorimeters, respectively.

The partial pressure of sulfur in covellite was measured by the dew-point method. CuS was sealed in an evacuated silica-glass tube and placed in a furnace. The end containing covellite was heated to the desired temperature, while the temperature of the other end was regulated until droplets of sulfur condensed on the inner wall. By narrowing the temperature interval between condensation and evaporation it was possible to determine the condensation temperature, and thus the vapor pressure of sulfur. The sulfur pressure at the condensation temperature was taken from Braune *et al.*⁽³²⁾

The temperature was measured with Pt-to-(Pt+10 mass per cent of Rh) thermocouples and the difference between measured and actual temperature was judged to be within 3 K. The dew-point was determined visually through a side-tube in the furnace.

3. Results and discussion

HEAT CAPACITY AND THERMODYNAMIC PROPERTIES

The experimental heat capacities of covellite for the low- and high-temperature ranges are given in chronological order in table 2 and presented graphically in

TABLE 2. Heat capacity of CuS; $M(\text{CuS}) = 95.606 \text{ g} \cdot \text{mol}^{-1}$; $R = 8.3144 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$

$\langle T \rangle$ K	$C_{p,m}$ R	$\langle T \rangle$ K	$C_{p,m}$ R	$\langle T \rangle$ K	$C_{p,m}$ R	$\langle T \rangle$ K	$C_{p,m}$ R	$\langle T \rangle$ K	$C_{p,m}$ R	$\langle T \rangle$ K	$C_{p,m}$ R
High-temperature measurements—University of Oslo											
Series I	390.67	6.045	502.08	6.370	730.54	7.014	637.93	6.718	775.98	8.607	
302.41	5.706	401.62	6.079	513.37	6.401	742.30	7.147	652.53	6.752	779.39	49.36
313.54	5.756	412.58	6.112	524.68	6.420			667.18	6.805	780.37	6023
324.62	5.792	423.57	6.146	536.00	6.456	Series III		681.86	6.844	781.45	56.89
335.68	5.833	434.72	6.170	547.30	6.514	551.76	6.524	696.40	6.896	789.69	7.702
346.72	5.891	445.90	6.209			565.99	6.567			804.27	7.666
357.74	5.939	457.10	6.247	Series II		580.26	6.596	Series IV		818.56	7.803
368.72	5.980	468.32	6.259	695.23	6.863	594.59	6.646	738.11	7.096	832.63	8.097
379.70	6.014	479.56	6.298	706.98	6.923	608.97	6.678	752.71	7.356		
		490.81	6.336	718.76	6.978	623.41	6.711	766.64	8.275		
Low-temperature measurements—University of Michigan											
Series V	129.98	4.059	196.78	4.999	Series VII	9.54	0.0873	25.77	0.7780		
50.98	1.906	140.12	4.247	207.22	5.096	318.95	5.785	10.61	0.1150	28.23	0.9021
55.00	2.106	150.32	4.414	217.60	5.189	329.17	5.850	11.71	0.1466	31.39	1.060
61.38	2.221	160.35	4.566	227.84	5.268	339.32	5.885	12.92	0.1845	35.08	1.241
66.69	2.401	170.31	4.703	237.94	5.341	347.42	5.932	14.08	0.2279	38.82	1.413
73.23	2.609	180.29	4.824	248.02	5.412			15.02	0.2638	42.95	1.599
81.32	2.864	190.33	4.934	258.13	5.474	Series VIII		16.23	0.3735	46.51	1.766
90.13	3.125	200.65	5.039	268.22	5.535	4.66	0.0111	17.78	0.3834	50.52	1.930
100.07	3.383			278.32	5.593	5.43	0.0197	19.51	0.4647	55.79	2.030
110.11	3.629	Series VI		288.52	5.648	6.69	0.0338	21.32	0.5533	61.13	2.214
120.07	3.855	186.52	4.892	298.73	5.703	7.61	0.0468	23.38	0.6567	66.94	2.411
						8.54	0.0636				

figure 1. The approximate temperature increments used in the determinations can usually be inferred from the adjacent mean temperatures in table 2.

The estimated standard deviation of a single heat-capacity measurement in the low-temperature region is about 1 per cent at 7 K, decreasing to 0.1 per cent over the range 30 to 300 K, and 0.2 per cent from 300 to 350 K. In the higher-temperature region it is about 0.3 per cent.

The experimental heat capacities for the low- and high-temperature regions were fitted to polynomials in temperature by the method of least squares. The fitting and especially the joins between the fitted segments were checked by inspection of a plot of $dC_{p,m}/dT$ against T . At the lowest temperatures the heat capacity was extrapolated assuming a linear $C_{p,m}/T$ against T^2 relation to $T \rightarrow 0$. Values of the thermodynamic functions were obtained from the polynomial expressions, by numerical integration using Simpson's rule,^(3,3) and from the observed enthalpy and entropy of decomposition. The values are presented in table 3 for selected temperatures. Within the decomposition region the heat capacity was estimated from large-scale plots.

The smoothed low-temperature heat capacities, compared with earlier work in the inset of figure 1, are somewhat lower than the values reported by Anderson.^(1,5) Excellent agreement between our values and the heat capacities by Ferrante *et al.*^(1,7)

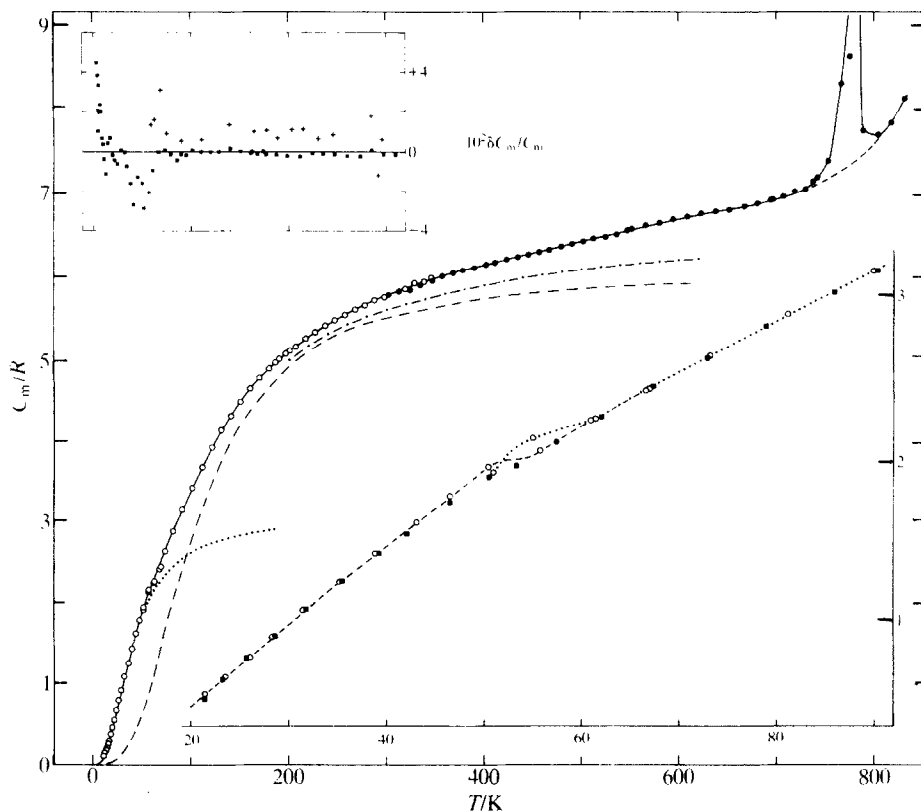


FIGURE 1. Heat capacity of CuS. \circ , Present values from the University of Michigan; \bullet , present values from the University of Oslo; ---, estimated $C_{v,m}$; - · -, estimated $C_{v,m} + C_m(d)$; ····, $C_{v,m}$ calculated from Debye's theory with $\Theta_D = 184$ K for a two-dimensional lattice; inset, fractional deviations from the present smoothed values of the earlier values: \blacksquare , Ferrante *et al.*⁽¹⁷⁾ +, Anderson.⁽¹⁵⁾

is observed above 70 K, whereas some scatter is present at lower temperatures. The resulting entropy $S_m^\circ(298.15 \text{ K}) = 8.100R$ is 0.3 per cent higher than the value of Ferrante *et al.*⁽¹⁷⁾ This is primarily caused by deviations near 50 K. Anderson obtained a value about 1.2 per cent lower⁽¹⁵⁾ due to uncertainties in extrapolation below 53 K. In the higher-temperature region the obtained values are up to 1 per cent higher than those of Ferrante *et al.*⁽¹⁷⁾

No heat-capacity peaks were observed in the temperature region between 8 K and the decomposition temperature. This is in agreement with the findings by Ferrante *et al.*⁽¹⁷⁾ but it contradicts Okamoto *et al.*⁽¹³⁾ who reported indistinct polymorphic phase transitions between 90 and 300 K. However, a small bump is observed around 55 K (see figure 1). This small effect was observed at a somewhat higher temperature in Series V than in Series VIII, which probably indicates that the previous thermal history is of importance. A similar but smaller bump was reported by Ferrante *et al.*⁽¹⁷⁾ The molar enthalpy connected with this effect is less than $0.8419R \cdot K$ using a reference heat capacity estimated by least-squares fitting of

TABLE 3. Thermodynamic properties of CuS; $M(\text{CuS}) = 95.606 \text{ g} \cdot \text{mol}^{-1}$;
 $R = 8.3144 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$

$\langle T \rangle$ K	$C_{p,m}$ R	$\Delta_0^T S_m$ R	$\Delta_0^T H_m$ R · K	$\Phi_m(T, 0)$ R	$\langle T \rangle$ K	$C_{p,m}$ R	$\Delta_0^T S_m$ R	$\Delta_0^T H_m$ R · K	$\Phi_m(T, 0)$ R
β-Phase									
10	0.0978	0.0350	0.2602	0.0089	298.15	5.695	8.101	1136.6	4.289
15	0.2628	0.1033	1.131	0.0279	300	5.703	8.136	1147.2	4.312
20	0.4882	0.2087	2.989	0.0592	320	5.794	8.507	1262.1	4.563
25	0.7393	0.3445	6.055	0.1022	350	5.911	9.031	1437.7	4.923
30	0.9876	0.5011	10.368	0.1555	375	5.997	9.442	1586.6	5.211
40	1.477	0.8527	22.712	0.2850	400	6.074	9.832	1737.6	5.488
50	1.886	1.229	39.640	0.4361	425	6.147	10.202	1890.3	5.754
60	2.199	1.601	60.101	0.5993	450	6.218	10.556	2044.9	6.011
70	2.496	1.962	83.563	0.7683	475	6.289	10.894	2201.2	6.259
80	2.825	2.317	110.22	0.9398	500	6.361	11.218	2359.4	6.499
90	3.117	2.667	139.95	1.112	525	6.436	11.530	2519.4	6.731
100	3.383	3.010	172.47	1.285	550	6.510	11.831	2681.1	6.956
120	3.852	3.669	244.97	1.628	575	6.583	12.122	2844.8	7.175
140	4.243	4.294	326.06	1.965	600	6.650	12.404	3010.2	7.387
160	4.562	4.882	414.22	2.293	625	6.710	12.677	3177.3	7.593
180	4.819	5.434	508.13	2.611	650	6.764	12.941	3345.8	7.794
200	5.031	5.954	606.71	2.920	675	6.819	13.198	3515.5	7.989
220	5.205	6.441	709.10	3.218	700	6.889	13.447	3686.9	8.180
240	5.356	6.901	814.73	3.506	725	7.005	13.690	3860.3	8.365
260	5.487	7.335	923.18	3.784	750	(7.102)	13.929	4036.6	8.547
280	5.601	7.746	1034.1	4.053	780.5	(7.334)	14.216	4256.6	8.763
Cu _{2-x} S(s) + S(l)									
780.5	(7.334)	16.971	6405.9	8.763	825	7.936	17.393	6744.2	9.218
800	(7.565)	17.155	6550.9	8.966					

polynomials to the heat capacities in the pre- and post-transitional regions. An attempt to resolve the observed heat capacity into contributions from lattice vibrations and electronic properties ($C_{\text{obs}} = C_l + C_e$) revealed the presence of an anomalous low-temperature behavior. The lattice heat capacity was estimated by extrapolating the constant-volume heat capacity in the harmonic approximation using a constant Debye temperature and adding a dilational heat-capacity term. The contribution from thermal expansion was estimated by the Grüneisen approximation:

$$C_m(d) = \{F\alpha C_{p,m} T / (1 + F\alpha T)\},$$

where α , the isobaric expansivity, is adequately described by $3.7 \times 10^{-5} \text{ K}^{-1}$ from 300 to 700 K,⁽³⁴⁾ and F the Grüneisen parameter, was assumed to be 2.0. The constant Debye temperature is often taken as the maximum of Θ_D in a plot of Θ_D against temperature. However such a maximum was not observed and the Debye temperature was estimated to be 420 K. The electronic heat capacity was then derived from the high-temperature heat capacity under the assumption that $C_e = \gamma T$ is a reasonable approximation even at higher temperatures. This led to $\gamma = 0.0045 \text{ J} \cdot \text{K}^{-2} \cdot \text{mol}^{-1}$, which is in keeping with the electric conductivity of CuS. (The magnetic contribution to the heat capacity is zero for diamagnetic covellite.)

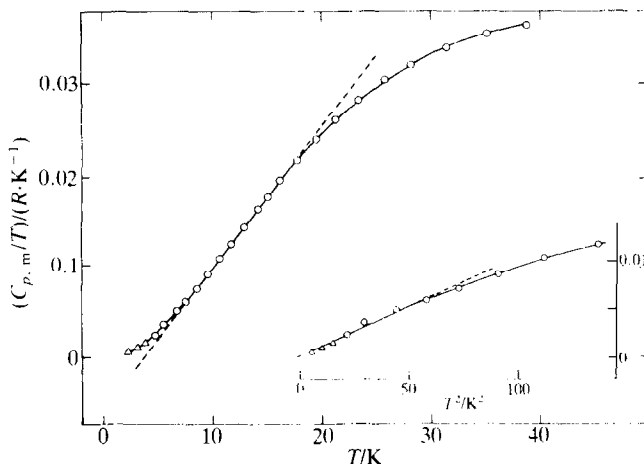


FIGURE 2. Plot of $C_{p,m}/T$ against T and against T^2 . Δ , Values read from figure 1 of Isino and Kanda.⁽¹⁶⁾

The calculated values of $C_{V,m}$ and $C_{p,m}$, indicated by dashed lines in figure 1, show that the agreement is poor in the low-temperature region (the dilational contribution is neglected at low temperatures). In figure 2, $C_{p,m}/T$ in the low-temperature region is plotted against T and against T^2 . It shows that $C_{p,m}$ is proportional to T^3 at very low temperatures (≈ 2 to ≈ 5 K) whereas it is proportional to T^2 in the region ≈ 5 to ≈ 20 K. Such behavior may be explained on the basis of the Debye theory of low-frequency modes of lattice vibrations with the assumption of a quasi-two-dimensional lattice. The anomaly might then originate from the weak bonding in the c -axis direction.⁽⁶⁾ Deviation from a Debye-type density of states, *e.g.* in form of a low-lying optical branch in the frequency distribution, might also contribute to the anomalous lattice heat capacity. These findings initiated a structural study which confirmed that changes in the structure occur around 55 K.⁽³⁴⁾ A coupling between the structural change and the reduced dimensionality is possible. Assuming a two-dimensional lattice, a constant-volume heat capacity was calculated in the low-temperature region using a constant Debye temperature by

$$C_{V,m}/R = 4(T/\Theta_D)^2 \int_0^{\Theta_D/T} \{x^3 e^x (e^x - 1)^{-2}\} dx,$$

which at very low temperatures may be approximated by letting the upper limit go to infinity giving

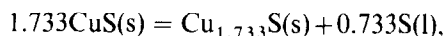
$$C_{V,m}/R = 28.848(T/\Theta_D)^2.$$

A two-dimensional Debye temperature for $T < 50$ K was evaluated from figure 2 and found to be 184 K. The resulting constant-volume heat capacity is indicated in figure 1. The failure of the T^2 relation for temperatures above 20 K may partly originate from failure of the continuum model and partly from excitations of higher-frequency lattice-vibration modes. This means that the lattice heat capacity at higher temperatures must be estimated in terms of a three-dimensional model. Below ≈ 5 K the T^2 relation does not hold, and a transition to T^3 behavior is

observed. Such a transition is also observed in graphite,^(35,36) where Komatsu⁽³⁷⁾ proposed that for sufficiently long phonon wavelengths, a weak shearing interaction between neighboring layers would play an important role. In covellite the picture is complicated by a transition to a superconductive phase at ≈ 1.6 K,⁽¹⁶⁾ and the origin of the T^3 relation is not clear. Experimentally determined frequency distributions are needed for solving these questions. The electronic heat capacity, extrapolated from the T^3 temperature region (see figure 2), was found to be zero within experimental-error limits. This fact may indicate changes in the electronic properties as a function of temperature, or more probably, show the difficulty in resolving the heat capacity of CuS into different contributions at these very low temperatures.

DECOMPOSITION

To evaluate the molar enthalpy and entropy changes during the decomposition reaction:



a reference non-transitional heat-capacity curve has been estimated. (The Cu-rich composition limit of digenite is taken from Rau.)⁽³⁸⁾ First of all, corrections for the enthalpy connected with vaporization of sulfur species from liquid sulfur had to be carried out. The dissociation pressure of covellite in the region from 680 K to the decomposition temperature has been determined.⁽¹⁸⁻²¹⁾ However, we also needed vapor pressures in the region above 780 K. These measurements were carried out by the dew-point method as described in section 2. The resulting values, as well as those from previous investigations, are presented graphically in figure 3. The temperature dependence of the equilibrium pressures may be represented by

$$\ln(p/\text{kPa}) = -36145 \text{ K}/T + 51.435, \quad 720 \text{ K} < T < 780 \text{ K},$$

$$\ln(p/\text{kPa}) = -4344 \text{ K}/T + 10.665, \quad 780 \text{ K} < T < 840 \text{ K}.$$

The observed pressures are about 84 and 60 per cent of the pressure over pure sulfur at 733 and 813 K, respectively. This lowering, which may partly be ascribed to a definite solubility of the sulfide in liquid sulfur, is greater than expected for an ideal mixture. The temperature dependence of the saturation pressure was taken from Braune *et al.*⁽³²⁾ To calculate the enthalpy of dissociation, the changes in the amounts of substance of the different gas species were calculated under the assumption of ideal-gas behavior. The vapor space in the silica container was derived from the total volume by subtracting the volumes of the silica glass ($\rho = 2.201 \text{ g} \cdot \text{cm}^{-3}$)⁽³⁹⁾ and of the covellite ($\rho = 4.68 \text{ g} \cdot \text{cm}^{-3}$) present.

The enthalpy of formation of the different sulfur-vapor species, $\text{S}_n(\text{g})$, $n > 2$, from liquid sulfur, at the temperature in question, was calculated from the heat-capacity equations and the values of $\Delta_f H_m^\circ(298.15 \text{ K})$ recommended by Mills.⁽⁴⁰⁾ The values for $\text{S}_2(\text{g})$ were taken from reference 41, whereas the heat capacity of S(s or l) was taken from West.⁽⁴²⁾ The resulting enthalpy of vaporization was at most 1.6 per cent of the total enthalpy increment for the sample due to an energy input. The smallness of the correction justifies the assumption of ideal-gas behavior and the neglect of the differences in the molar heat capacity of S between liquid sulfur and the different gas

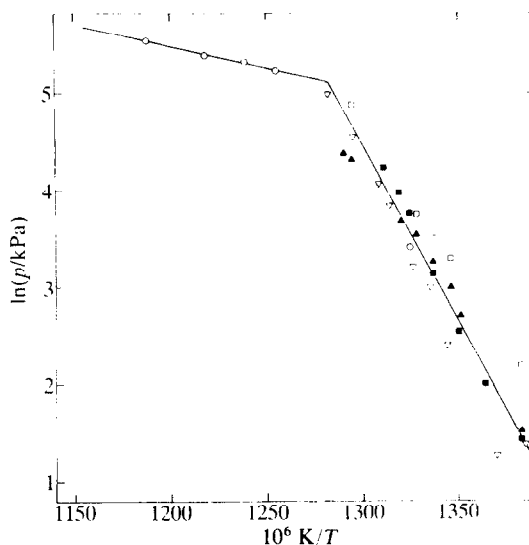


FIGURE 3. Plot of $\ln(p/\text{kPa})$ against $1/T$. \circ , Present values; ∇ , Dickson *et al.*;⁽²¹⁾ \blacksquare , Allen and Lombard;⁽²⁰⁾ \square , Preuner and Brockmoller;⁽¹⁹⁾ \blacktriangle , Wasjuchnowa.⁽¹⁸⁾

species. The reference non-transitional heat-capacity curve was estimated by least-squares fitting of polynomials to the corrected heat capacities in the pre- and post-transitional regions. The background is indicated by the broken line in figure 1, whereas the results of the transformation evaluations are given in table 4. The molar enthalpy and entropy of decomposition are $2149.3R \cdot \text{K}$ and $2.755R$.

The anomalous heat capacity in the post-decomposition region might originate from changes in the sulfur-rich-phase limit of the high-digenite field. However, according to the phase diagram presented by Rau the sulfur-rich-phase limit changes only from $\text{Cu}_{1.7500}\text{S}$ at 780 K to $\text{Cu}_{1.7509}\text{S}$ at 840 K. The unknown heat capacity of liquid sulfur in this temperature region precludes a closer analysis of the heat-capacity rise.

TABLE 4. Enthalpy of decomposition of CuS ; $M(\text{CuS}) = 95.606 \text{ g} \cdot \text{mol}^{-1}$;
 $R = 8.3144 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$

$\langle T \rangle$ K	$C_{p,m}$ R	$C_{p,m}(\text{non-trs.})$ R	ΔT K	$\Delta_{\text{dis}} H_m$ R · K	$\Delta_{\text{dec}} H_m$ R · K	$\Delta_{\text{dec}} S_m$ R
Series IV, Run 2-9						
752.712	7.356	7.127	14.362	0.563	2.72	0.0036
766.368	8.275	7.221	13.490	0.765	13.45	0.0176
775.983	8.607	7.296	5.199	0.716	6.10	0.0079
779.389	49.36	7.320	1.625	0.064	68.26	0.0876
780.370	6023	7.332	0.326	0.010	1963.6	2.5162
781.451	56.89	7.339	1.842	0.053	91.22	0.1167
789.451	7.702	7.421	14.625	0.402	3.72	0.0047
804.27	7.666	7.633	14.520	0.243	0.25	0.0003
					2149.3	2.755
$T_{\text{dec}} = 780.5 \text{ K}$						

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