Report of Investigations 7691

Low-Temperature Heat Capacities and High-Temperature Enthalpies of Sodium Chromate

By M. J. Ferrante, J. M. Stuve, and M. P. Krug
Albany Metallurgy Research Center, Albany, Oreg.

MARCH 3, 1849

UNITED STATES DEPARTMENT OF THE INTERIOR
Rogers C. B. Morton, Secretary

BUREAU OF MINES
Elburt F. Osborn, Director

The work upon which this report is based was done under an agreement between the Bureau of Mines, U.S. Department of the Interior, and the U.S. Atomic Energy Commission.

This publication has been cataloged as follows:

Ferrante, Michael J

Low-temperature heat capacities and high-temperature enthalpies of sodium chromate, by M. J. Ferrante, J. M. Stuve, and M. P. Krug. [Washington] U.S. Dept. of the Interior, Bureau of Mines [1972]

12 p. illus., tables. (U.S. Bureau of Mines. Report of investigations 7691)

Includes bibliography.

Based on work done in cooperation with the U.S. Atomic Energy Commission.

1. Sodium chromate. I. Stuve, John M., jt. auth. II. Krug, Marion P., jt. auth. III. Title. (Series)

TN23.U7 no. 7691 622.06173

U.S. Dept. of the Int. Library

CONTENTS

ILLUSTRATIONS

TABLES

LOW-TEMPERATURE HEAT CAPACITIES AND HIGH-TEMPERATURE ENTHALPIES OF SODIUM CHROMATE

by

M. J. Ferrante,[1] J. M. Stuve,[1] and M. P. Krug[2]

ABSTRACT

Low-temperature heat capacities and high-temperature enthalpies were determined calorimetrically for Na_2CrO_4. A reversible transition was found at 700° K with an isothermal heat of transition of 2,263 cal/mole. High-temperature X-ray diffraction analysis showed that the transition was a crystal change from the low-temperature orthorhombic form to the high-temperature hexagonal form. At 795° K the hexagonal form had the parameters a_o = 5.691 and c_o = 7.478 A. Powder diffraction data for the high-temperature form are given and possible structures discussed. The melting point was determined to be 1,065° K with a heat of fusion of 5,810 cal/mole. Enthalpy and entropy increments from this investigation were combined with other data from the literature to calculate enthalpies of formation, free energies of formation, and equilibrium constants of formation from 298° to 1,400° K. Equations that represent enthalpies above 298° K are given.

INTRODUCTION

This Bureau of Mines investigation was made to determine thermodynamic properties for Na_2CrO_4 over an extended temperature range. The research was done in cooperation with the Atomic Energy Commission, as a part of the fast-breeder reactor program, to provide thermochemical data for a portion of the Na-Cr-O system.

The experimental work involved two areas of calorimetric investigation: Low-temperature heat capacities were determined with an adiabatic calorimeter over the temperature range of 5.5° to 308.5° K, and high-temperature enthalpy increments were determined with a drop calorimeter between 298° and 1,192° K. No similar data have appeared previously in the literature.

The high-temperature investigation of Na_2CrO_4 showed a reversible transition at 700° K. Flach (4)[3] reported this temperature to be 686° K. X-ray

---

[1] Research chemist.

[2] Research physicist.

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

diffraction studies showed this transition to be a reversible crystal change and provided data for the crystal form above the transition temperature. The melting point was determined to be 1,065° K, in confirmation of the temperature reported by Flach (4) and Hartford (6).

The present results were combined with an enthalpy of formation at 298.15° K, given by Nelson, Moss, and Hepler (12), to provide a table that lists the principal thermodynamic properties for both the crystal and liquid states.

MATERIALS

Anhydrous Na_2CrO_4 was prepared by heating reagent-grade $Na_2CrO_4 \cdot 4H_2O$. The tetrahydrate was first heated at 110° C for about 4 days with occasional grinding and stirring. The temperature was then increased to 480° C, where it was maintained for 3 hr. The X-ray diffraction pattern of the product matched that given in the ASTM Catalog of X-ray Powder Data for anhydrous, orthorhombic Na_2CrO_4. Wet chemical analysis gave 32.11 pct chromium as compared with the theoretical chromium content of 32.10 pct. Optical emission spectroscopy showed that the sample contained between 10 to 100 ppm silicon as the only detected impurity.

EXPERIMENTAL WORK AND DISCUSSION OF RESULTS

The results of calorimetric determinations are expressed in defined calories (1 cal = 4.1840 j). Molecular weights were calculated from the 1969 Table of Atomic Weights (9). Temperatures from 5° to 20° K were based on the National Bureau of Standards P2-20 (1965) Provisional Scale; from 20° to 90° K, on the National Bureau of Standards 1955 Scale; and from 90° to 1,200° K, on the International Practical Temperature Scale of 1968 (IPTS-68).

Low-Temperature Heat Capacities

Heat-capacity determinations were made with an adiabatic calorimeter. Only a brief description of this newly constructed apparatus will be given here since a detailed report on the construction and operation of the calorimeter will be published in the near future. This apparatus consists of a liquid nitrogen-liquid helium cryostat capable of cooling a 90-ml sample to 5° K. Sample temperatures are measured with a germanium resistance thermometer between 5° and 15° K, and a platinum resistance thermometer from 15° to 310° K. Both thermometers were calibrated by the National Bureau of Standards. Temperatures were determined potentiometrically with a double, six-dial microvolt potentiometer. Adiabatic control of the shielding system is operated automatically by electronic circuitry capable of discriminating temperature differences as small as 0.0005° K. Electrical energy input to the sample is supplied by a precision regulated constant current source and measured by a high-impedance integrating digital voltmeter. A small amount of helium gas ($\sim 10^{-5}$ mole) is usually introduced into the sample container prior to determinations to facilitate heat exchange. The heat capacity of the empty calorimeter is about 0.01 cal/deg at 6° K and 9 cal/deg at 300° K.

Experimental heat capacities, determined with a 125.15-g sample of Na_2CrO_4, are listed in table 1 and shown graphically in figure 1. No anomalous behavior or transitions were found. The estimated error is the larger of either ±0.0005 cal/deg or 0.1 pct of the measured heat capacity for the range of 9° to 300° K.

TABLE 1. - Experimental heat capacities of Na_2CrO_4(c)

T, ° K	C_p, cal/deg mole	T, ° K	C_p, cal/deg mole
5.515	0.0166	63.626	11.577
5.872	.0208	67.782	12.429
6.206	.0260	72.041	13.257
6.594	.0331	76.384	14.093
7.088	.0438	80.637	14.913
7.665	.0593	77.675	14.331
8.322	.0810	79.936	14.769
9.028	.1098	84.217	15.577
9.771	.1471	89.071	16.436
10.564	.1954	94.820	17.345
11.466	.2612	102.216	18.458
12.421	.3430	111.115	19.739
13.330	.4332	120.763	21.028
14.247	.5369	130.960	22.309
15.275	.6479	141.377	23.451
16.287	.7896	152.047	24.547
17.456	.9675	163.101	25.568
18.748	1.184	174.634	26.563
20.009	1.406	186.520	27.478
21.383	1.675	198.564	28.348
23.369	2.081	210.657	29.319
26.014	2.664	222.751	30.037
29.521	3.498	234.928	30.743
33.940	4.570	247.061	31.439
39.135	5.862	259.169	32.087
44.799	7.246	271.101	32.679
48.017	8.015	283.161	33.312
50.182	8.548	295.158	33.858
52.837	9.154	306.839	34.381
55.979	9.847	308.466	34.457
59.592	10.692		

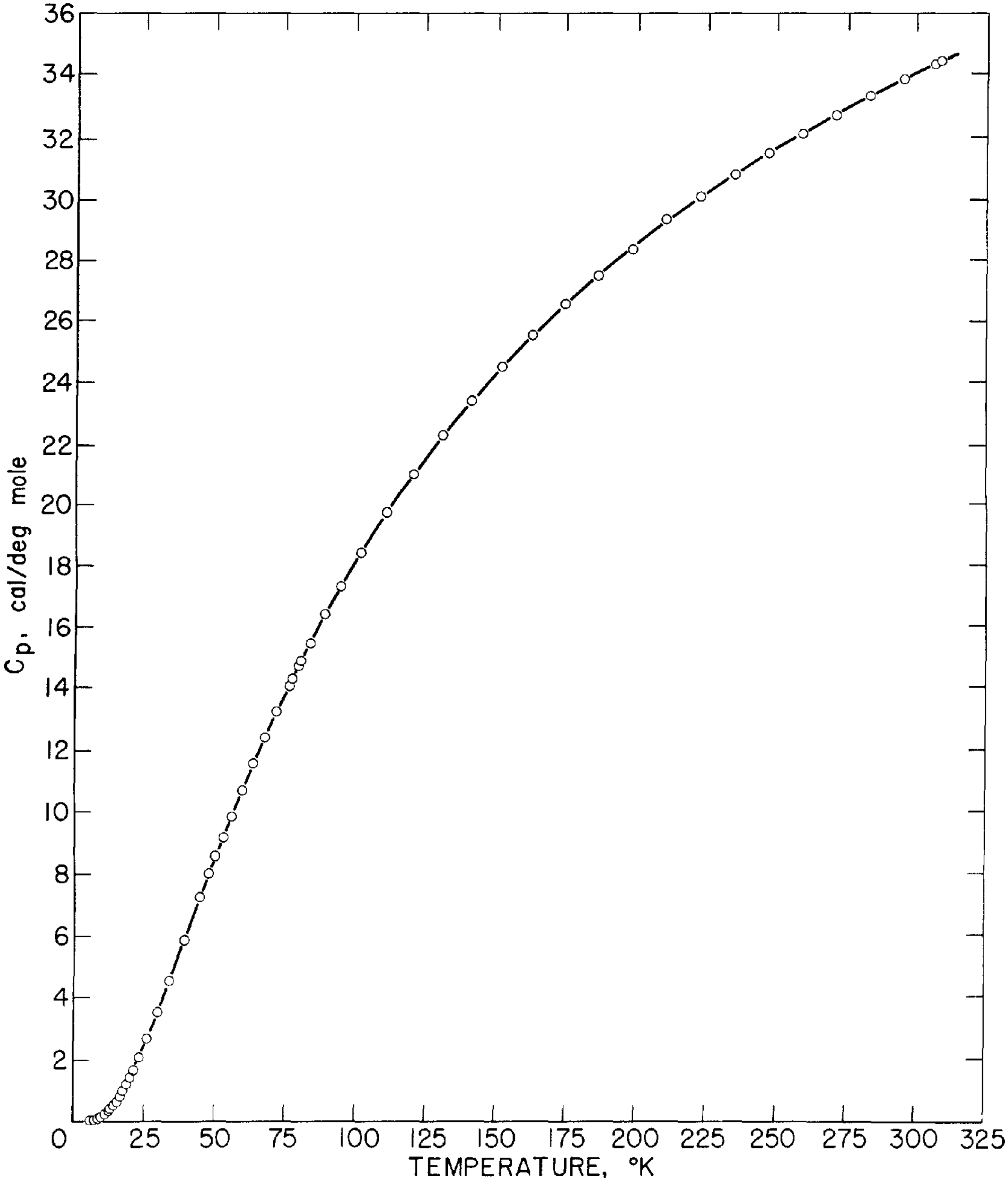

FIGURE 1. - Low-Temperature Heat Capacity.

Table 2 lists the smoothed heat capacity values at regular temperature intervals. These values were obtained from polynomial functions (5, 10), which were fitted to the experimental data with the aid of a computer. Table 2 also shows the derived thermodynamic quantities S°, $-(G°-H°_0)/T$, and $H°-H°_0$.

TABLE 2. - Low-temperature thermodynamic properties of Na_2CrO_4(c)[1]

T, °K	C_p	S°	$-(G°-H°_0)/T$	$H°-H°_0$, cal/mole
	cal/deg mole			
5	(0.012)	(0.003)	(0.001)	(0.013)
10	.160	.043	.009	.337
15	.620	.184	.040	2.159
25	2.435	.884	.219	16.627
30	3.610	1.430	.374	31.698
40	6.073	2.808	.804	80.19
50	8.460	4.421	1.363	152.90
60	10.747	6.168	2.017	249.05
70	12.868	7.986	2.739	367.28
80	14.804	9.833	3.510	505.8
90	16.559	11.679	4.315	662.7
100	18.150	13.508	5.143	836.4
110	19.599	15.307	5.986	1,025.3
120	20.927	17.070	6.836	1,228.0
130	22.149	18.794	7.690	1,443.5
140	22.278	20.477	8.543	1,670.7
150	24.324	22.119	9.394	1,098.7
160	25.293	23.720	10.240	2,156.9
170	26.190	25.281	11.079	2,414.4
180	27.021	26.802	11.910	2,680.5
190	27.793	28.283	12.733	2,954.6
200	28.513	29.728	13.547	3,236.1
210	29,190	31,135	14.351	3,524.7
220	29.831	32.508	15.145	3,819.8
230	30.445	33.848	15.929	4,121.2
240	31.036	35.156	16.703	4,428.6
250	31.605	36.435	17.467	4,741.9
260	32.149	37.685	18.221	5,061
270	32.665	38.908	18.964	5,385
280	33.148	40.105	19.698	5,714
290	33.603	41.276	20.422	6,048
298.15	33.968	42.212	21.005	6,323
300	34.052	42,423	21.136	6,386

[1] Values in parentheses are extrapolations.

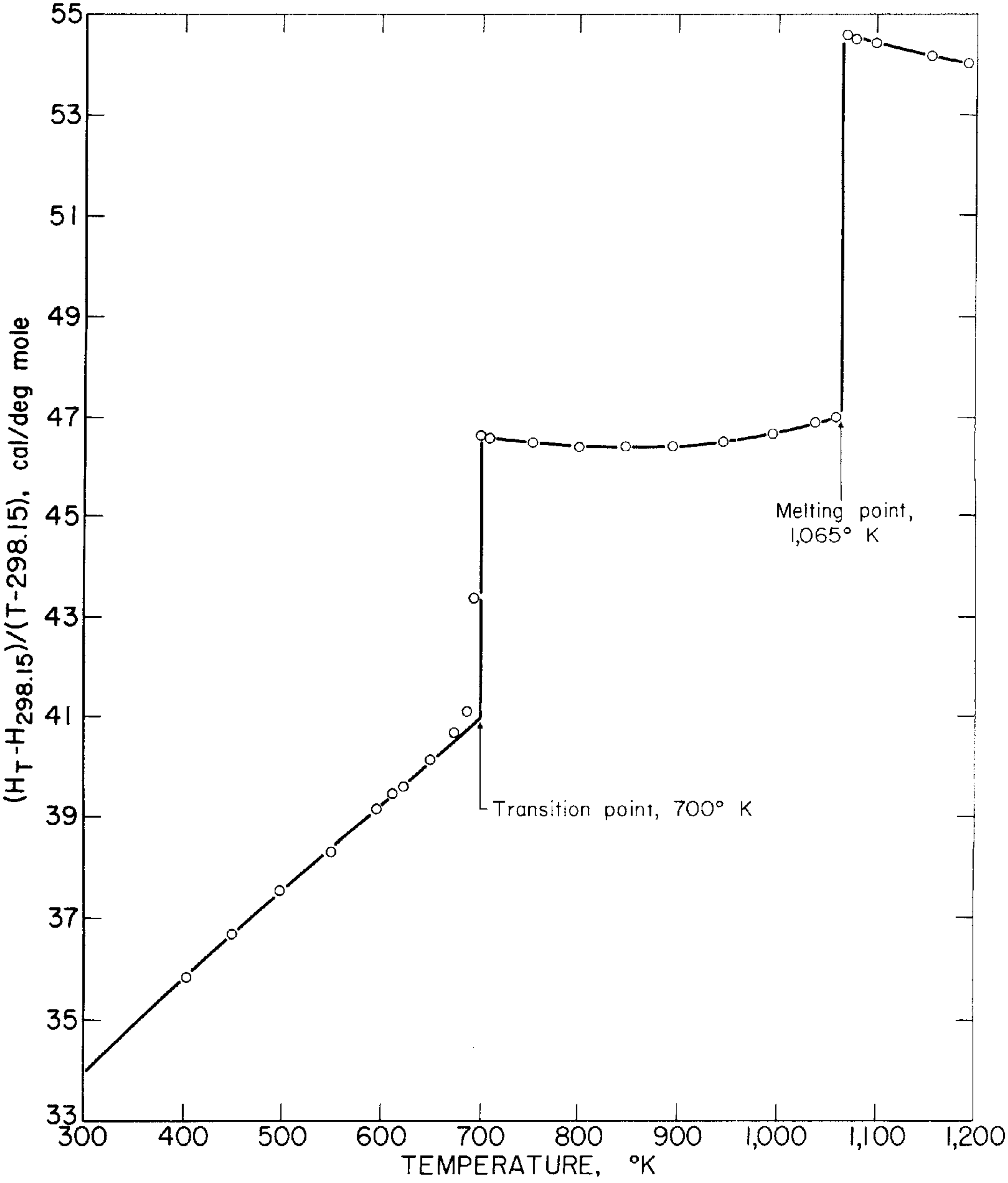

FIGURE 2. - High-Temperature Enthalpy Function.

High-Temperature Enthalpies

Enthalpy determinations above 298.15° K were made with the copper-block drop calorimeter described by Douglas and King (1). This apparatus was modified by the use of a six-dial microvolt potentiometer in conjunction with a precision electronic null detector.

Platinum-rhodium alloy capsules served as sample containers. Enthalpies of the empty capsules were determined in separate experiments. Two capsules were filled with Na_2CrO_4 samples of 8.3145 and 8.5485 g. The second capsule filling was to establish the curve of the enthalpy function in the liquid state after the first capsule had developed a leak.

Experimental enthalpy values relative to 298.15° K are listed in table 3 and plotted in figure 2 as the function $(H°-H°_{298.15})/(T-298.15)$ against temperature. The standard error is 0.07 pct for the determinations, and the absolute uncertainty of enthalpy is estimated to be ±0.3 pct.

TABLE 3. - Experimental enthalpies above 298.15° K of Na_2CrO_4(c,l)

T, ° K	$H°-H°_{298.15}$, cal/mole	T, ° K	$H°-H°_{298.15}$, cal/mole
403.1	3,759	753.4	21,161
449.5	5,557	799.1	23,243
498.0	7,503	847.1	25,470
547.2	9,544	893.9	27,653
596.4	11,676	945.3	30,088
611.6	12,366	994.9	32,508
622.7	12,850	1,039.1	34,740
649.9	14,120	1,059.8	35,790
673.4	15,267	1,069.9	42,120
686.8	15,970	1,078.7	42,540
693.8	17,159	1,098.3	43,557
700.2	18,751	1,155.2	46,420
709.8	19,167	1,191.6	48,258

Results of the enthalpy determinations showed a rapidly reversible transition at 700° K with an isothermal heat of transition of 2,263 cal/mole. No previous value was found in the literature for the heat of transition. Flach (4) reported the temperature of transition to be 686° K. X-ray diffraction studies below and above the transition point were conducted. Discussion of these X-ray studies is presented in the next section.

The temperature and heat of fusion were also determined by the enthalpy experiments. No previous value was found in the literature for the heat of fusion, which is 5,810 cal/mole. The melting point of 1,065° K agrees with the temperature reported by Flach (4) and Hartford (6). The temperature range required for complete melting was less than 10°. This behavior indicated that the Na_2CrO_4 crystals were unusually free of structural defects. X-ray diffraction analysis showed that a melted sample reverted completely to the room-temperature orthorhombic form after quenching in the calorimeter.

Polynomial functions (5, 10) were fitted to the experimental enthalpy values with the aid of a computer. During this procedure, the high-temperature enthalpy data were found to merge smoothly with the low-temperature heat-capacity data given in table 2. The resulting polynomial functions were used to calculate enthalpies above 298° K at 100° intervals (table 4). Heat capacities, entropies, and free energy functions also are given in table 4, in which all of the low- and high-temperature experimental results have been combined. Constancy of the heat capacity for the liquid state permitted confident extrapolation of data to 1,400° K.

TABLE 4. - Thermodynamic properties of $Na_2CrO_4(c,l)$[1]

$[2Na(c,l) + Cr(c) + 2O_2(g) = Na_2CrO_4(\alpha,\beta,l)]$

T, ° K	C_p	S°	$-(G°-H°_{298.15})/T$	$H°-H°_{298.15}$	$-\Delta Hf°$	$-\Delta Gf°$	Log Kf
	cal/deg mole			kcal/mole			
0	0	0	∞	-6.323	-	-	-
100	18.150	13.508	68.378	-5.487	-	-	-
200	28.513	29.728	45.163	-3.087	-	-	-
298.15	33.968	42.212	42.212	0	318.600	293.039	214.803
300	34.052	42.423	42.213	.063	318.597	292.881	213.364
[2]371	36.63	49.920	42.987	2.572	318.506	286.806	168.952
371	36.63	49.920	42.987	2.572	319.748	286.806	168.952
400	37.62	52.714	43.591	3.649	319.700	284.231	155.297
500	40.95	61.467	46.311	7.578	319.335	275.396	120.376
600	44.41	69.235	49.495	11.844	318.679	266.664	97.132
[3]700(α)	48.14	76.357	52.831	16.468	317.710	258.068	80.572
700(β)	45.54	79.589	52.831	18.731	315.447	258.068	80.572
800	45.84	85.678	56.564	23.291	314.585	249.931	68.278
900	47.20	91.145	60.107	27.934	313.678	241.900	58.741
1,000	49.63	96.235	63.468	32.767	312.629	233.982	51.137
[4]1,065(β)	51.78	99.425	65.565	36.061	311.831	228.897	46.972
1,065(l)	50.44	104.881	65.565	41.871	306.021	228.897	46.972
1,100	50.44	106.512	66.842	43.637	305.611	226.369	44.975
1,200	50.44	110.901	70.333	48.681	304.493	219.210	39.924
1,300	(50.44)	(114.938)	(73.611)	(53.725)	(303.472)	(212.157)	(35.667)
1,400	(50.44)	(118.676)	(76.699)	(58.768)	(302.542)	(205.175)	(32.029)

[1] Values in parentheses are extrapolations.

[2] Melting point of Na.

[3] Transition point of Na_2CrO_4.

[4] Melting point of Na_2CrO_4.

The following standard-form equations were derived by Kelley's method (11) to represent the smoothed enthalpies given in table 4. To conform to general usage, the equations express enthalpies as calories per mole. It should be noted that enthalpy values calculated from the simplified standard-form equations are only approximations and should not be considered as precise as the values given in table 4. Both the percent average deviations of these equations from the smoothed data and temperature ranges of validity are given in parentheses.

The alpha, beta, and liquid forms of the equation are as follows:

$$\alpha: \quad H^\circ - H^\circ_{298.15} = 24.40T + 16.81 \times 10^{-3}T^2 + 0.41 \times 10^5 T^{-1} - 8{,}907$$

(<0.1 pct; 298°-700° K),

$$\beta: \quad H^\circ - H^\circ_{298.15} = 1.03T + 20.35 \times 10^{-3}T^2 - 78.51 \times 10^5 T^{-1} + 19{,}254$$

(<0.1 pct; 700°-1,065° K), and

$$1: \quad H^\circ - H^\circ_{298.15} = 50.44T - 11{,}848$$

(<0.05 pct; 1,065°-1,400° K).

X-Ray Diffraction Studies

To better characterize the transition at 700° K, powder X-ray diffraction data were taken at temperatures above and below this temperature. No previous high-temperature X-ray data could be found in the literature. The X-ray sample of Na_2CrO_4 was deposited by evaporation from a benzene slurry onto a a platinum strip heater that was mounted on the lower unit of a special high-temperature diffractometer attachment. Because of the unreactive nature of the sample, the vacuum cover assembly was not required. The study was made on a horizontal diffractometer with copper K-alpha radiation. Temperature was determined by means of a thermocouple attached by spot welding to the back of the strip heater.

Na_2CrO_4 was found to transform from the room-temperature orthorhombic structure to a high-temperature hexagonal structure. At 795° K the hexagonal structure has the parameters $a_0 = 5.691$, and $c_0 = 7.478$ A ($c/a = 1.314$). The data are presented in table 5. The transition was found to be rapid and completely reversible; a pattern made at 525° K immediately after rapidly cooling from 795° K showed only the room-temperature form. The transition was accompanied by a reversible change in the visual appearance of the sample from bright yellow at room temperature to reddish brown at 795° K.

TABLE 5. - X-ray powder data for Na_2CrO_4 at 795° K with copper K-alpha radiation $\lambda = 1.54178$ A

d(obs), A	d(calc), A	I(obs)	hkl	d(obs), A	d(calc), A	I(obs)	hkl
4.955	4.929	20	100	2.2251	2.2244	5	103
4.133	4.115	80	101	2.0561	2.0576	28	202
3.740	3.739	12	002	1.8675	1.8695 1.8628	5	004 210
2.980	2.979	40	102				
2.853	2.846	100	110	1.8095	1.8076	8	211
2.468	2.464	15	200	1.6681	1.6674	8	212
2.2653	2.2644	8	112	1.6429	1.6429	8	300

Several sulfates and a few mixed salts have been reported to have unit cells of approximately the aforementioned dimensions. Wyckoff (13) gives three closely related hexagonal structures for compounds with this formula type: (1) The $LiKSO_4$ structure type with space group $P6_3$ (No. 173); (2) the Al_2BaO_4 structure type with space group $P6_322$ (No. 182); and (3) the aphthitalite or glaserite structure type, $KNaSO_4$ to $K_3Na(SO_4)_2$, with space group $P\bar{3}ml$ (No. 164). More recently, Fischmeister (3) has described a similar structure with the space group $P6_3/mmc$ (No. 194) for a high-temperature form of Na_2SO_4 (type I). This structure differs from the others in that the anions are centered on the special positions ±(2/3, 1/3, 1/4), but anions in adjacent unit cells are rotated by 60° with respect to each other in a more or less random fashion.

In the high-temperature Na_2CrO_4 pattern, hhl and 001 reflections were not observed for odd values of l. One cannot be certain from powder data, but, if these are actual extinctions, No. 194 is the only one of the aforementioned space groups that would fit the high-temperature form of Na_2CrO_4. There is some similarity between the intensities in the powder patterns of Na_2CrO_4 and Na_2SO_4, but there is too much difference in scattering powder of chromium and sulfur ions for such a comparison to be conclusive. Thus, it seems likely that Na_2CrO_4 at high temperatures has the structure of Na_2SO_4 (type I).

ENTHALPIES AND FREE ENERGIES OF FORMATION

Enthalpies of formation, free energies of formation, and equilibrium constants of formation were calculated from 298° to 1,400° K by combining the enthalpies and entropies determined in this investigation with supplementary data. The enthalpy of formation at 298° K was taken from Nelson, Moss, and Hepler (12). Enthalpy and entropy data for sodium were obtained from Hultgren, Orr, Anderson, and Kelley (8). Similar information for chromium metal was taken from Hultgren (7), and for gaseous oxygen, from JANAF tables (2). Where necessary, the auxiliary data were corrected to IPTS-68. The results of these calculations are listed in table 4 as $-\Delta Hf°$, $-\Delta Gf°$, and Log Kf.

SUMMARY

This investigation provides new low-temperature heat-capacity data and high-temperature enthalpy data for Na_2CrO_4. A reversible transition at 700° K was shown to be a crystal transformation from orthorhombic to hexagonal. X-ray powder diffraction data of the hexagonal form are presented. The determination of the melting point at 1,065° K is in agreement with the one reported by Flach (4) and Hartford (6).

REFERENCES[4]

1. Douglas, T. B., and E. G. King. High-Temperature Drop Calorimetry. Ch. 8 in Experimental Thermodynamics, v. 1, Calorimetry of Non-Reacting Systems, ed. by J. P. McCullough and D. W. Scott. Butterworths, London, 1968, pp. 293-331.

2. Dow Chemical Company, Thermal Research Laboratory. JANAF Thermochemical Tables. Supp. 370-1, National Technical Information Service, Springfield, Va., August 1966.

3. Fischmeister, H. F. Röntagenkristallographische Ausdehnungsmessungen an einigen Alkalisulfaten. Ein Beitrag zur Kenntnis der Anionenfehlordung im Na_2SO_4 I-Typ (X-ray Crystallographic Dimensional Measurements of Some Alkali Sulfates. Anionic Disorder in Na_2SO_4 Type I). Monatsh. Chem., v. 93, 1962, pp. 420-434.

4. Flach, E. Kaliumchromat und Natriumchromat, ihr Fähigkeit zur Mischkristall- und Doppelsalzbildung und ihre Beziehungen zu den entsprechenden Sulfaten (Potassium and Sodium Chromates; Mixed Crystals and Double Salt; Relation to the Corresponding Sulphates). Inaugural Dissertation, Univ. of Leipzig, 1912. Abstract available for examination at the Albany Metallurgy Research Center, Bureau of Mines, Albany, Oreg.

5. Forsythe, G. E. Generation and Use of Orthogonal Polynomials for Data-Fitting With Digital Computer. J. Soc. Ind. and Appl. Math., v. 5, 1957, pp. 74-88.

6. Hartford, W. H. Properties of Technically Important Hexavalent Chromium Compounds. Ind. and Eng. Chem., v. 41, 1949, pp. 1993-1997.

7. Hultgren, R. Private communication, July 1970. Available for examination at the Albany Metallurgy Research Center, Bureau of Mines, Albany, Oreg.

8. Hultgren, R., R. L. Orr, P. D. Anderson, and K. K. Kelley. Selected Values of Thermodynamic Properties of Metals and Alloys. John Wiley & Sons, Inc., New York, 1963, 963 pp.

9. International Union of Pure and Applied Chemistry, Division of Inorganic Chemistry, Commission on Atomic Weights. Atomic Weights of the Elements (1969). Pure and Appl. Chem., v. 21, 1970, pp. 91-108.

10. Justice, Bruce H. Thermal Data Fitting With Orthogonal Functions and Combined Table Generation. The FITAB Program. Univ. of Michigan, Ann Arbor, Mich. COO-1149-143, 1969, 49 pp.

---

[4] Titles enclosed in parentheses are translations from the language in which the item was originally published.

11. Kelley, K. K. Contributions to the Data on Theoretical Metallurgy. XIII. High-Temperature Heat-Content, Heat-Capacity, and Entropy Data for the Elements and Inorganic Compounds. BuMines Bull. 584, 1960, 232 pp.

12. Nelson, T., C. Moss, and L. G. Hepler. Thermochemistry of Potassium Permanganate, Potassium Molybdate, Potassium Chlorate, Sodium Chlorate, Sodium Chromate, and Sodium Dichromate. J. Phys. Chem., v. 64, 1960, pp. 376-377.

13. Wyckoff, R. W. G. Crystal Structures. Interscience Publishers, New York, v. 3, 1965, pp. 112-116.

U.S. GOVERNMENT PRINTING OFFICE: 1972—708-894:535

BIBLIOGRAPHIC DATA SHEET

1. Report No.
BuMines RI 7691

2.

3. Recipient's Accession No.
PB-213 876

4. Title and Subtitle
Low-Temperature Heat Capacities and High-Temperature Enthalpies of Sodium Chromate

5. Report Date
November 1972

6. Performing Organization Code

7. Author(s)
M. J. Ferrante, J. M. Stuve, and M. P. Krug

8. Performing Organization Rept. No.

9. Performing Organization Name and Address
Albany Metallurgy Research Center
Bureau of Mines, USDI
P.O. Box 70
Albany, OR 97321

10. Project/Task/Work Unit No.

11. Contract/Grant No.

12. Sponsoring Agency Name and Address
Division of Metallurgy
Bureau of Mines
U.S. Department of the Interior
Washington, DC 20240

13. Type of Report & Period Covered
Research, 6-70/6-72

14. Sponsoring Agency Code

15. Supplementary Notes

16. Abstracts
Low-temperature heat capacities and high-temperature enthalpies were determined calorimetrically for NA2CRO4. A reversible trnasition was found at 700 deg K with an isothermal heat of transition of 2,263 cal/mole. High-temperature X-ray diffraction analysis showed that the transition was a crystal change from the low-temperature orthorhombic form to the high-temperature hexagonal form. At 795 deg K the hexagonal form had the parameters ao = 5.691 and co = 7.478 A. Powder diffraction data for the high-temperature form are given and possible structures discussed. The melting point was determined to be 1,065 deg K with a heat of fusion of 5,810 cal/mole. Enthalpy and entropy increments from this investigation were combined with other data from the literature to calculate enthalpies of formation, free energies of formation, and equilibrium constants of formation from 298 to 1,400 deg K. Equations representing enthalpies above 298 deg K are given.

17. Key Words and Document Analysis. 17a. Descriptors
Thermodynamic properties
Heat capacity
Entropy
Enthalpy
X-ray diffraction

17b. Identifiers/Open-Ended Terms

17c. COSATI Field/Group 07D

18. Distribution Statement
Release unlimited by NTIS.

19. Security Class (This Report)
UNCLASSIFIED

20. Security Class (This Page)
UNCLASSIFIED

21. No. of Pages
~~12~~ 17

22. Price
[redacted]