

of N-Cl bond while the perpendicular mean square amplitudes of N-F and N-Cl bonds are widely different. The ζ values obtained in this investigation show that the Coriolis coupling between different modes of vibration is rather weak. However, there exists fairly strong coupling between N-Cl symmetric and N-Cl antisymmetric stretching modes of vibration as well as between the FNCl symmetric and FNCl antisymmetric bending modes of vibration.

One of the authors (B. S. N.) is grateful to the University Grants Commission for the award of a scholarship.

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THERMAL EXPANSION OF CADMIUM MOLYBDATE

THE present study of thermal expansion of cadmium molybdate is a part of our programme of "X-ray studies on scheelite-type compounds". We have already reported the results on the precision determination of lattice parameters and thermal expansion of KIO_4 ¹, NaIO_4 ², SrWO_4 ³, BaWO_4 ⁴ and CaMoO_4 ⁵. A perusal of literature shows that except for some room temperature lattice parameter data, there is no work on their temperature variation for CdMoO_4 .

Small chips of cadmium molybdate crystals, obtained from Dr. R. R. Soden of the Bell Telephone Laboratories, U.S.A., were crushed into powder form to fill the specimen cup of the back-reflection-focussing camera.⁶ The experimental technique employed and the procedure used in the evaluation of accurate values of the lattice parameters, their standard errors and the coefficients of thermal expansion are essentially the same as described in earlier publications.³⁻⁵ The reflections which were unambiguously indexed and employed in calculating the values of the a and c parameters were $(2.2.12)_{a_1a_2}$, $(3.3.10)_{a_1a_2}$, $(620)_{a_1a_2}$ and $(536)_{a_1a_2}$. The lattice parameters obtained at different temperatures are given in Table I and are shown in Fig. 1.

TABLE I
Lattice parameters of CdMoO_4 at different temperatures

Temperature °C.	a Å	c Å
30	5.1559 $\pm 0.0004^*$	11.1950 $\pm 0.0020^*$
70	5.1580	11.2035
105	5.1588	11.2059
165	5.1625	11.2202
210	5.1645	11.2278
265	5.1671	11.2367
310	5.1697	11.2443
355	5.1729	11.2558

* Standard errors as calculated by Jette and Foote method.⁷

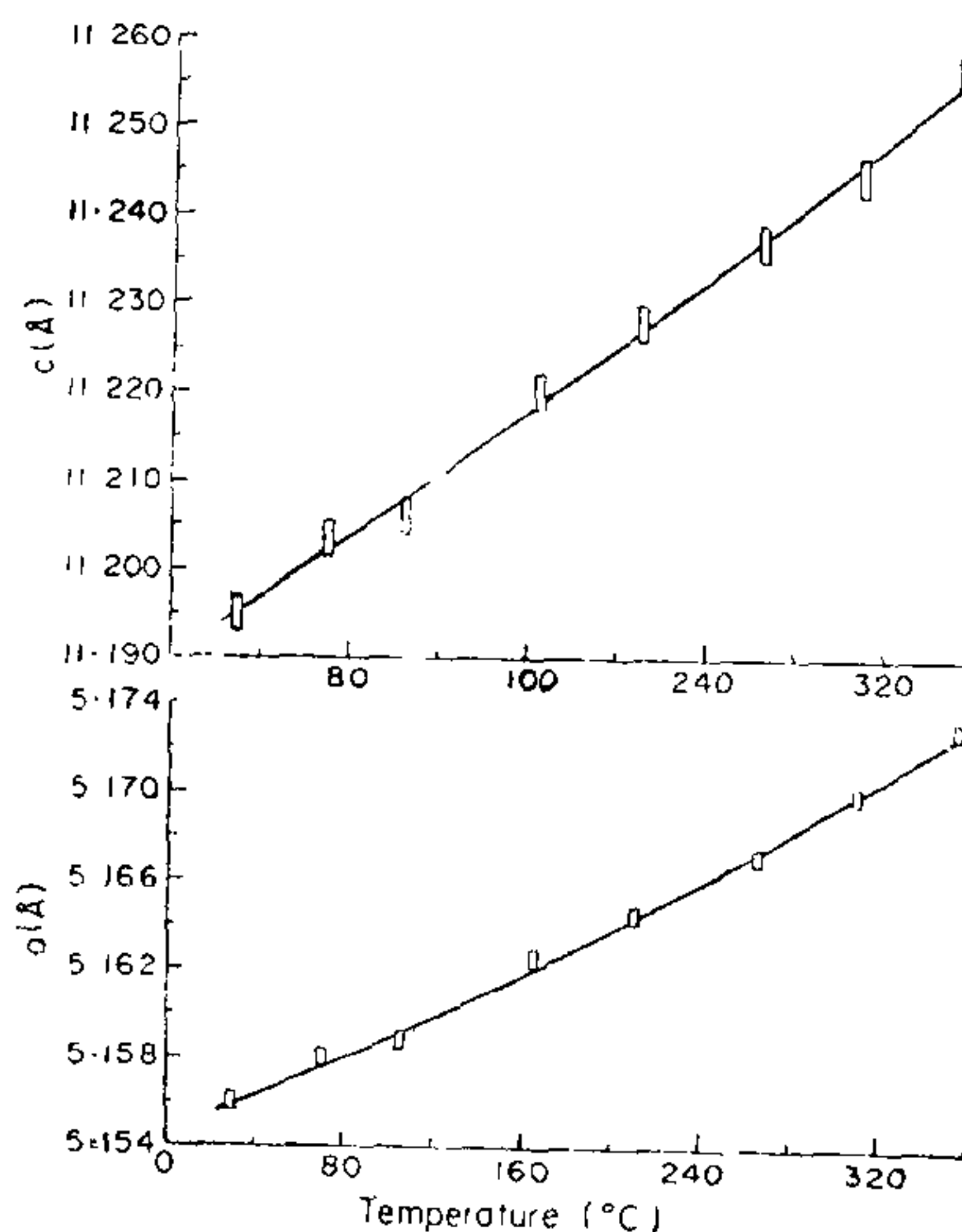


FIG. 1. Temperature variation of the lattice parameters of CdMoO_4 .

Least-square fitting of the temperature-parameter data gave the following expressions for the temperature dependence of a and c .

$$a_t = 5.1548 + 38.38 \times 10^{-6}t + 33.40 \times 10^{-9}t^2$$

$$c_t = 11.1903 + 164.19 \times 10^{-6}t + 48.10 \times 10^{-9}t^2$$

Here a_t and c_t are the two parameters in Å units at temperature $t^\circ\text{C}$.

The values, of the two principal coefficients of expansion α_a along a -axis and α_c along c -axis, at different temperatures, calculated from the temperature-parameter plots are given in Table II.

TABLE II
Coefficients of thermal expansion of CdMoO_4
at different temperatures

Temp. (°C.)	$\alpha_a \times 10^6$		$\alpha_c \times 10^6$	
	Obs.	Calc.	Obs.	Calc.
30	..	6.85	..	15.13
40	7.27	7.09	15.28	15.21
60	7.47	7.56	15.41	15.37
100	8.34	8.45	15.63	15.72
140	9.21	9.29	16.44	16.10
200	10.38	10.42	16.53	16.75
240	11.25	11.10	16.97	17.22
300	11.93	12.01	18.13	18.00
340	12.88	12.53	18.54	18.56
350	..	12.66	..	18.70

The temperature dependence of the coefficients could be expressed by the following equations:

$$\alpha_a = 6.10 \times 10^{-6} + 25.43 \times 10^{-9} t - 19.15 \times 10^{-12} t^2$$

$$\alpha_c = 14.91 \times 10^{-6} + 7.00 \times 10^{-9} t + 10.98 \times 10^{-12} t^2$$

where t is in °C. The values of α_a and α_c calculated by using these two equations are also given in Table II.

In Table III the lattice parameters of CdMoO_4 obtained at room temperature are compared with a few others available in literature. There is good agreement between the present values and those reported by Swanson *et al.*⁹

TABLE III
Lattice parameters of CdMoO_4 at room
temperature

Authors	a Å	c Å
Donnay and Nowacki ⁸	.. 5.148 ±0.003	11.17 ± 0.02
Swanson <i>et al.</i> ⁹	.. 5.155	11.194
Chichagov <i>et al.</i> ¹⁰	.. 5.17	11.19
Present study	.. 5.1559 ±0.0004	11.1950 ± 0.0020

It is worth a mention that in CdMoO_4 , the coefficients of expansion along the tetragonal axis is larger than that along the a -axis and remains larger throughout the temperature range covered, a feature observed in other scheelite-type crystals also.

The authors wish to express their thanks to Dr. R. R. Soden of the Bell Telephone Laboratories for kindly supplying cadmium molybdate crystals used in the present investigation. One of us (S. V. S.) thanks the Ministry of Education, Government of India, for financial assistance.

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K-ABSORPTION SPECTRUM OF 1-AMIDINO-2-THIOUREA COMPLEX OF NICKEL (II)

RECENTLY several workers¹⁻⁷ have studied the electronic structure of transition metal complexes and have correlated their results obtained from the X-ray absorption spectroscopy with magnetic measurements. In the present paper, the authors have studied the K-absorption spectrum of a freshly prepared chelate of nickel⁸(II), viz., nickel (II) complex of 1-amidino-2-thiourea, Ni (ATU)_2 and have attempted to correlate the observed results with the structure proposed by Paigankar.⁹

A 40 cm. focussing spectrograph of Cauchois type mentioned elsewhere¹⁰ was used in this investigation. The (201) and (100) planes of mica which served as the diffracting crystal gave a dispersion of about 12 X.U. mm.⁻¹ in the first order. A sealed X-ray tube with copper target was operated at 10 KV and 6 mA. Exposure times varied from 40 to 50 hours on the ORWO X-ray films.

Absorbing screens were prepared by pressing the compound between two thin mylar sheets. After several trials screens of suitable thicknesses were obtained which gave maximum contrast in the absorption spectra. The screens were placed in between the crystal holder and the photographic plate. A microphotometer $M_{\phi 4}$ both recording and the direct reading type was used in this investigation.