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The crystal and molecular structure of π-allyl-dihydrobis-(3,5-dimethyl-1-pyrazolyl)boratodicarbonylmolybdenum, $H_2B[(CH_3)_2pz]_2Mo(CO)_2C_3H_5$: addendum.

By C. A. KOSKY, *Polymer Research Institute, Polytechnic Institute of Brooklyn, New York* 11201, *U.S.A.* and P. GANIS and G. AVITABILE, *Università di Napoli, Istituto Chimico,* 80134 *Napoli, Italy*

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The following line should be inserted between N(1′) and C(1) in the table of thermal parameters (Table 3) in a recent article under the above title (Kosky, Ganis & Avitabile, 1971):

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
N(2′)	2·660 (0·207)	2·632 (0·212)	2·796 (0·209)	−0·252 (0·167)	1·020 (0·173)	0·870 (0·169)

Reference

KOSKY, C. A., GANIS, P. & AVITABILE, G. (1971). *Acta Cryst.* B27, 1859.

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Phase transformation of thin caesium iodide layers at low temperatures.

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A low-temperature tetragonal phase of thin caesium iodide crystalline layers detected below −140°C by means of electron diffraction is described. The lattice parameters are $a=3{\cdot}88$ and $c=4{\cdot}12$ Å. The linear thermal expansion coefficient of the CsCl-type B_2 phase as determined in the temperature range between +20°C and −140°C was $4{\cdot}96\times10^{-5}$.

In connexion with investigations of the structural properties of thin ionic crystals by means of electron diffraction, a phase transformation of the CsCl-type B_2 caesium iodide has been detected at approximately −140°C.

The specimens supplied by British Drug Houses were prepared in a Balzers 350-G vacuum device at $2{\cdot}0\times10^{-5}$ torr by evaporation from a molybdenum boat, and then investigated in a cold-stage specimen holder, developed in our laboratory, with a Zeiss EF-4 electron-optical equipment between +20 and −150°C at 50 kV. The $L\lambda$ values, where L is the tube length and λ is the electron beam wave length, were determined with a TlCl standard.

Fig. 1. represents the temperature dependence of the lattice constant of the B_2 structure. The linear thermal expansion in the temperature range between +20°C and −140°C was fitted by the least-squares method. Accordingly the value $4{\cdot}96\times10^{-5}$ was obtained.

It was found that the Debye–Scherrer diagrams taken at $t<-140$°C showed, beside the ordinary reflexions of

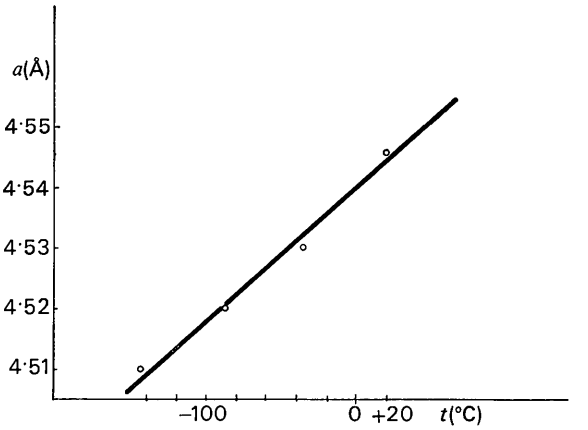

Fig. 1. Dependence of the lattice constant on temperature in B_2-type caesium iodide.

Table 1. *Low-temperature data*

Number of the Debye–Scherrer ring	Ring diameter D (*mm*)	d(Å) measured	Intensity	*hkl*	d(Å) calculated
1	7·038	3·901	strong	200	3·873
2	7·510	3·650	strong	101	3·638
3	7·977	3·442	faint	210	3·464
4	13·323	2·060	faint	002	2·060
5	14·372	1·910	strong	321	1·905
6	18·109	1·516	faint	510	1·519
7	21·246	1·290	faint	203 }	1·294 }
				600 }	1·291 }

the B_2-type CsI, a number of partly well-developed, and partly-faint lines not present in the diffraction patterns of the specimen at room temperature.

Though the reproducibility is not very good the low-temperature reflexions could be easily determined by assuming a tetragonal lattice (Table 1). The lattice parameters may approximately be defined as $a=3{\cdot}88$ and $c=4{\cdot}12$ Å.

One unit cell accommodates two formula units; the coordinates of the ions in the unit cell may be

$$\begin{array}{ll} I^- & 0, \tfrac{1}{2}, \tfrac{1}{2}; \tfrac{1}{2}, 0, \tfrac{1}{2} \text{ or} \\ & 0, \tfrac{1}{2}, 0; \tfrac{1}{2}, 0, 0 \end{array}$$

$$\begin{array}{ll} Cs^+ & 0, 0, 0; \tfrac{1}{2}, \tfrac{1}{2}, 0 \text{ or} \\ & 0, 0, \tfrac{1}{2}; \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}. \end{array}$$

On heating to room temperature the tetragonal reflexions disappeared. A similar transformation is well known with NH_4Br (Ketelaar, 1934).

The author wishes to thank Professor I. Náray–Szabó for his helpful interest, and Mrs L. Fülöp and Miss L. Rudnyánszky for their help in carrying out the experiments.

Reference

KETELAAR, I. (1934). *Nature, Lond.* **134**, 251.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England).

Protein data bank

It is proposed to establish a repository system for protein crystallographic data operated jointly by the Crystallographic Data Centre, Cambridge, England (sponsored by the Office for Scientific and Technical Information) and the Brookhaven National Laboratory, U.S.A. The system will be responsible for the storage of atomic coordinates, structure factors and electron density maps and will make these data available on request. Distribution will, whenever possible, be on magnetic tape in machine-readable form. There will be no charge for the service other than handling costs. Files will be updated as new material is received. Annual announcement of the total holding will be made in the organic bibliographic volumes of the reference series *Molecular Structures and Dimensions* published for the Crystallographic Data Centre and the International Union of Crystallography by Oosthoek's, Utrecht, The Netherlands.

The success of the proposed system will depend on the response of the protein crystallographers supplying data. These will be accepted either 'raw' or refined, in machine-readable form or as manuscripts. It would be helpful if laboratories intending to join the scheme would communicate in the first instance with Mrs Olga Kennard or Dr D. G. Watson at the University Chemical Laboratories, Lensfield Road, Cambridge, England, who are responsible for the organization of the system. Data can be submitted to Cambridge, England, or to Dr W. C. Hamilton at the Brookhaven National Laboratory, Upton, New York 11973, U.S.A., where the data will be computer processed.

The two centres will maintain identical files and both will provide data services. It should be emphasized that the proposed data bank is intended to supplement existing publication media, and depositing material in it should not be regarded as a substitute for the publication of the results of structural investigations in a scientific journal.

Radiation safety in X-ray diffraction and spectroscopy

A conference on radiation safety in X-ray diffraction and spectroscopy was held at the University of Pennsylvania, Philadelphia, Pennsylvania, U.S.A., 6–7 January 1970, to fill the need for improved communications between users of X-ray diffraction and spectroscopy equipment, health physicists, and government agencies with regulatory responsibilities. Radiation safety in the use of the equipment was discussed from the viewpoints of experimentalists and other users, individuals concerned primarily with radiation safety, and agencies responsible for developing and enforcing guides, standards and regulations. A report of the proceedings has now been published; it includes the papers presented and also the discussions held at the conference. Copies are available from the Superintendent of Documents, U.S.Government Printing Office, Washington, D.C. 20402, U.S.A. The price is U.S. $2.00 per copy.