Title
THE CRYSTAL STRUCTURE OF INDIUM (I) IODIDE

Authors
Jones, Robert E.
Templeton, David H.

Publication Date
1955-08-03

UCRL 3088

UNIVERSITY OF CALIFORNIA

Radiation Laboratory

THE CRYSTAL STRUCTURE OF INDIUM (I) IODIDE

DISCLAIMER

UCRL-3088
Unclassified Physics

UNIVERSITY OF CALIFORNIA
Radiation Laboratory
Berkeley, California

Contract No. W-7405-eng-48

THE CRYSTAL STRUCTURE OF INDIUM (I) IODIDE

Robert E. Jones and David H. Templeton

August 3, 1955

Printed for the U. S. Atomic Energy Commission

The Crystal Structure of Indium (I) Iodide

Robert E. Jones and David H. Templeton
Department of Chemistry and Radiation Laboratory
University of California, Berkeley, California

August 3, 1955

Crystals of InI were grown by heating indium with a slight excess of iodine in an evacuated tube at 300° C. The vapor condensed on a cooler surface outside the furnace as brownish-red, plates of the {010} form. From Weissenberg and powder photographs taken with CuKα and CrKα radiation an orthorhombic unit cell was found with dimensions:

$a = 4.75$ Å, $b = 12.76$ Å, $c = 4.91$ Å (each $\pm 0.2\%$).

For Z = 4, the density is calculated as 5.39 compared with 5.32 measured by Klemm and Dierks (1934). The absences correspond to space groups Cmcm, Cmc2, and C2cm. Agreement with the intensities is found with the TlI-type structure (Helmholz, 1936), space group Cmcm (D_{2h}^{17}) with the atoms in positions 4(c) (International Tables, 1952): $\pm(0, y, 1/4) + (0, 0, 0; 1/2, 1/2, 0)$.

The atomic parameters were determined by sharpened $(F_o - F_c)$ syntheses for the projection along [001], computed only along the y axis. The hk0 intensities were estimated visually and corrected for Lorentz and polarization factors and for absorption. For allowed reflections the intensity is independent of h for constant k and ℓ, except for the factors dependent on θ. Sets of corrected intensities with $\ell = 0$ and with the same value of k were plotted versus $\sin^2\theta$, and sharpened F^2 values, corresponding to point atoms at rest, were read from these curves at an arbitrary $\sin^2\theta$. This procedure was adopted to improve the accuracy of the absorption corrections. The best fit was obtained with $y = 0.398 \pm 0.001$ for indium and 0.145 ± 0.001 for iodine. The standard deviations are according to the method of Cox and Cruikshank (1948).

Each atom has one neighbor of the opposite kind at 3.23 Å and four more at 3.46 Å. Two additional neighbors at 3.95 Å can hardly be considered nearest neighbors. The shortest In-In and I-I distances are 3.58 and 4.44 Å, respectively. The ionic radius of In^+, if this compound can be considered a salt, may be estimated as 1.32 Å if one uses the polymorphism of TlI (Helmholz, 1936; Barth, 1927) to calculate the distance In and I would have in the CsCl-type structure if it existed. One obtains essentially the same result using either Pauling's (1942) or Zachariasen's (1950) scheme for correcting for coordination if one uses the corresponding source for the radius of I^-.

The compound InBr has this same structure (Stephenson and Mellor, 1950). From the distances in this compound one can calculate in the same way essentially the same value for the radius by either scheme.

This research was supported by the U.S. Atomic Energy Commission.

Barth, T. (1927). Z. phys. Chem. 131, 105.

Cox, E.G., and Cruikshank, D.W.J. (1948). Acta Cryst. 1, 92.

Helmholz, L. (1936). Z. Krist. 95, 129.

International Tables for X-ray Crystallography (1952). Birmingham: Kynoch Press.

Klemm, W., and Dierks, F. (1934). Z. anorg. allgem. Chem. 219, 42.

Pauling, L. (1942). The Nature of the Chemical Bond 2nd ed. Cornell: University Press.

Stephenson, N.C., and Mellor, D.P. (1950). Australian J. Sci. Research A3, 581.

Zachariasen, W.H. (1950). Amer. Crystallog. Ass., Abstracts of Meeting at Penn. State Coll., 29.