Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

Acta Cryst. (1967). **23**, 1096

X-ray study of monothiourea-cadmium sulphate dihydrate crystal.

By S. NATARAJAN, *Department of Physics, Indian Institute of Technology, Madras* 36, *India*

(*Received* 19 *May* 1967)

Work on the structure of monothiourea-cadmium sulphate dihydrate was started in connexion with an investigation of crystal structures of some of the metallic complexes of thiourea to study the sulphur bridging in coordination compounds.

The crystals of monothiourea-cadmium sulphate dihydrate are transparent rectangular plates. The *a* axis was chosen along the length, the *b* axis parallel to the width, and the *c* axis along the thickness of the plates. These crystals cleave perfectly and easily in a plane perpendicular to *b* axis.

Rotation and Weissenberg photographs were taken about *a* and *b* axes with unfiltered copper radiation. The unit cell was found to be orthorhombic, with edges $a=7.88$, $b=13.70$, and $c=16.15$ Å. These lattice parameters were measured from *a*- and *b*-axis zero layer Weissenberg photographs and refined by Taylor, Sinclair, Nelson & Riley's extrapolation method.

The conditions limiting the possible reflexions, as obtained from the zero and higher layer Weissenberg photographs taken about *a* and *b* axes, led to the space group *Pcab* (D_{2h}^{15}) without any ambiguity. The density calculated on the basis of eight molecules per unit cell agrees well with the measured value.

Experimental

A structure was derived by Patterson methods and refined by difference synthesis and least squares. *R* indices of 0.18 for the 0*kl* reflexions and 0.32 for the *h*0*l* reflexions were obtained. Three-dimensional work was started but was discontinued when the author learned that an essentially similar structure had been derived by Cavalca, Domiano, Fava Gasparri & Boldrini (1967).

The author wishes to express his gratitude to Dr E. M. Gopalakrishna and Dr B. V. R. Murty of the Physics Department, I.I.T., Madras, for their encouragement in this work. Because there was an overlap in the work, Prof. L. Cavalca was kind enough to send a preprint of his work on the same crystal for comparison; and, the author wishes to express his thanks to him for this gesture.

References

CAVALCA, L., DOMIANO, P., FAVA GASPARRI, G. & BOLDRINI, P. (1967). *Acta Cryst.* **22**, 878.

Acta Cryst. (1967). **23**, 1096

Anomalous scattering corrections for X-rays. β-Radiations.

By A. C. HAZELL, *Department of Inorganic Chemistry, University of Aarhus,* 8000 *Aarhus, Denmark*

(*Received* 30 *May* 1967)

The real and imaginary components of the anomalous scattering corrections have been calculated for elements $Z=10$ (Ne) to $Z=98$ (Cf) for the following $K\beta_1$ radiations: Cr, Mn, Fe, Co, Ni, Cu, Zn, Mo, Rh, Pd, and Ag, by the method of Parratt & Hempstead, using the oscillator strengths calculated by Cromer.

Introduction

The total atomic scattering factor, *f*, is in general complex and given by

$$f=f_0+\Delta f'+i\Delta f'',$$

where f_0 is the Fourier transform of the electron distribution and $\Delta f'$ and $\Delta f''$ are the real and imaginary components of the anomalous scattering correction. The imaginary term is positive and corresponds to an advance in phase of the scattered radiation.

The use of anomalous scattering in the solution of the phase-problem is limited by the number of X-ray targets available. By using β radiations as well as α radiations the number of available wavelengths is increased. The lower intensity of the β radiations is compensated for in some cases by the larger values of $|\Delta f|$ which can be obtained; *e.g.* for Cu with Cu $K\beta$ radiation $\Delta f'=-4{\cdot}6$.

In the solution of centrosymmetric structures by the comparison of data collected with two wavelengths (Ramaseshan, Venkatesan & Mani, 1957; Caticha-Ellis, 1962; Hazell, 1964) it is possible (Hazell, 1966) to use the α and β radiations from the same target to obtain the two sets of data and to use the known ratio (calculated from the ratio *in vacuo* or determined experimentally) between the inten-