

If N is half-integral it follows that p_m is also half-integral, but there are $2p_m$ lattice points in every n th row of unit cells of the generating lattice. With this slight change in the significance of n , and with the

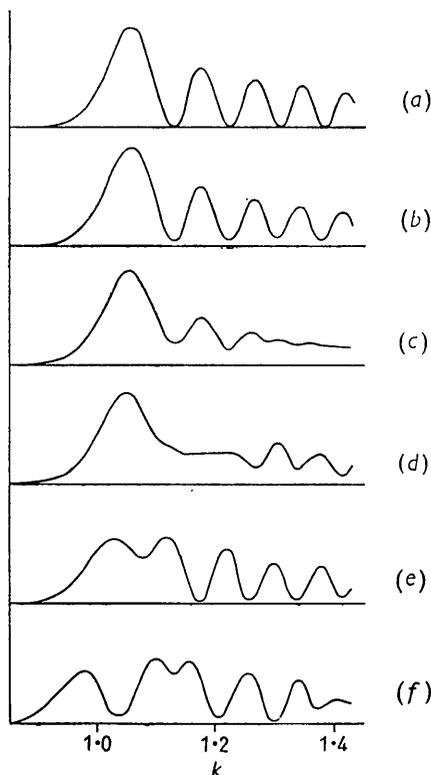


Fig. 1. $J^2_{p_m - Nl}(kp_m) + J^2_{p_m + Nl}(kp_m)$ for $p_m = 65$ and the following values of Nl : (a) 0; (b) 0.5; (c) 1.0; (d) 1.5; (e) 2.5; (f) 5.0. In order to correspond strictly with the diffracted intensity from a single layer of a helical cylindrical lattice, p_m should be half-integral when Nl is half-integral; but no appreciable difference is produced in the curves by a change of 0.5 in p_m .

summation with respect to ν extended to cover the range $1 \leq \nu \leq 2p_m$, all the formulae of § 3 are valid, and the conditions for the diffracted amplitude to be non-zero remain true. (When it is non-zero the amplitude is, of course, double that from a primitive lattice; analytically this arises from doubling the range of the summation over ν .) However, the condition

$$q = Kp_m \mp Nl$$

includes the condition that $K+l$ be even, since only integral values of q are involved in the expansion

$$\exp(ix \cos \theta) = J_0(x) + \sum_{q=1}^{\infty} i^q \cos q\theta J_q(x).$$

The restriction on the indices therefore arises analytically from a restriction on the orders of the Bessel functions, instead of in the usual way by the cancelling of trigonometric terms of opposite sign. Physically, of course, the restriction arises in precisely the same way as usual.

It is evident on general grounds that centred cylindrical lattices of the type c_n (Whittaker, 1955c) will diffract in exactly the same way as a primitive lattice, except that $h00$ reflexions will occur only when h is a multiple of n .

I wish to thank the Directors of Ferodo Ltd for permission to publish this paper.

References

- JAGODZINSKI, H. & KUNZE, G. (1954). *Neues Jb. Miner. Mh.* p. 137.
 WASER, J. (1955). *Acta Cryst.* 8, 142.
 WHITTAKER, E. J. W. (1954). *Acta Cryst.* 7, 827.
 WHITTAKER, E. J. W. (1955a). *Acta Cryst.* 8, 261.
 WHITTAKER, E. J. W. (1955b). *Acta Cryst.* 8, 265.
 WHITTAKER, E. J. W. (1955c). *Acta Cryst.* 8, 571.

Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

Acta Cryst. (1955). 8, 729

Determination of the absolute configuration of optically active complex ion $[\text{Coen}_3]^{3+}$ by means of X-rays. By YOSHIHIKO SAITO, KAZUMI NAKATSU, MOTOO SHIRO and HISAO KUROYA, *Institute of Polytechnics, Osaka City University, Minami-Ogimachi, Osaka, Japan*

(Received 2 June 1955)

The absolute configuration of optically active tri-ethylene-diamine cobalt (III) complex ion has been determined using the absorption-edge technique (Bijvoet,

Peerdeman & van Bommel, 1951). Hitherto unrecorded double salts having the composition $2D\text{-}[\text{Coen}_3]\text{Cl}_3 \cdot \text{NaCl} \cdot 6\text{H}_2\text{O}$ and $2L\text{-}[\text{Coen}_3]\text{Cl}_3 \cdot \text{NaCl} \cdot 6\text{H}_2\text{O}$ (en: ethylenedi-

amine, $\text{NH}_2\text{-CH}_2\text{-CH}_2\text{-NH}_2$) have been prepared, and, using Fe $K\alpha$ radiation ($\lambda = 1.937 \text{ \AA}$), their crystal structure has been completely determined by us (Shiro, Nakatsu, Saito & Kuroya, 1955) except for the 'hand'. The space group is $C_3^1\text{-}P3$ with one formula unit in a cell of dimensions

$$a = 11.47, c = 8.06 \text{ \AA}.$$

The structure belongs very nearly to the space group $C_3^1\text{-}P6_3$ in that all the atoms except one sodium and one chlorine per asymmetric unit are arranged according to the symmetry of $P6_3$.

In order to distinguish between $I(hkil)$ and $I(hk\bar{i}\bar{l})$, the latter being equivalent to $I(\bar{h}k\bar{i}\bar{l})$ because of pseudo symmetry when l is even, use was made of Cu $K\alpha$ radiation ($\lambda = 1.542 \text{ \AA}$), which can just excite the cobalt atoms ($\lambda_K = 1.608 \text{ \AA}$) in the crystal. It is more convenient to compare $I(hkil)$ with $I(hk\bar{i}\bar{l})$, since these two reflexions can be observed on the same oscillation photograph taken around the c axis and various correction factors come out exactly the same for these two reflexions. There are many such pairs of reflexions for which slight but discernible differences in intensities were observed, whereas no such differences were found when Fe $K\alpha$ radiation was used. It was also found that the inequality relations observed for one crystal are the reverse of those found for its enantiomorph. This observation strongly suggests that these differences are due to the anomalous dispersion of cobalt atoms in the crystal. In Table 1 observed and calculated relations between $I(hkil)$ and $I(hk\bar{i}\bar{l})$ are compared for 30 pairs only, of the lower orders. The visual estimates of the last two columns are the results of observations by a few persons independently. The calculated values are based on the structure model determined by us. The concordance, in general, of inequality signs in the observed and calculated intensities seen in the table indicates that the drawing of

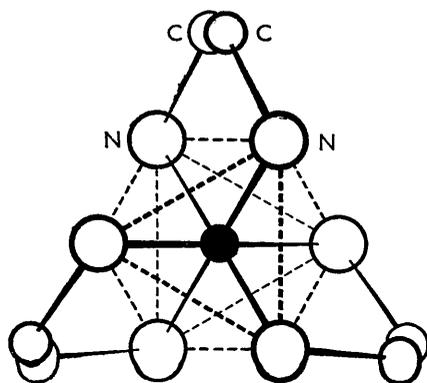


Fig. 1. Drawing of the $d(+)\text{-}[\text{Co}(\text{en})_3]^{3+}$ complex ion. Six nitrogen atoms form a slightly distorted octahedron around the central cobalt atom. The five-membered cobalt-ethylenediamine ring is not planar; each ethylenediamine ligand takes the so-called 'gauche' form.

Table 1. Observed and calculated intensities

hkl	Calculated*		Observed†	
	$I(hkil)$	$I(hk\bar{i}\bar{l})$	D form	L form
20 $\bar{2}2$	155	277	<	>
30 $\bar{3}2$	74	162	<	>
4042	1110	1010	? >	? <
50 $\bar{5}2$	396	382	?	?
70 $\bar{7}2$	209	201	?	?
11 $\bar{1}2$	1	133	<	>
21 $\bar{1}2$	3700	3450	>	<
3142	323	440	<	>
41 $\bar{1}2$	18	31	<	>
61 $\bar{1}2$	42	39	>	<
12 $\bar{3}2$	71	150	<	>
22 $\bar{4}2$	38	157	<	>
32 $\bar{5}2$	142	87	>	<
42 $\bar{6}2$	308	329	?	?
52 $\bar{7}2$	0.2	14	<	>
62 $\bar{8}2$	90	81	? <	? >
1342	946	893	? >	? <
23 $\bar{5}2$	465	521	? <	? >
3362	121	147	? <	? >
5382	84	75	? >	? <
6392	189	170	? >	? <
14 $\bar{5}2$	775	701	? >	? <
24 $\bar{6}2$	110	98	? >	? <
3472	34	48	? <	? >
4482	3	27	? <	? >
5492	98	106	? <	? >
15 $\bar{6}2$	315	297	>	<
2572	16	18	? <	? >
3582	143	134	? >	? <
2792	72	64	? >	? <

* Model shown in Fig. 1. The correction factors to be applied to the real and imaginary parts of the scattering factor of the cobalt atom for Cu $K\alpha$ radiation on account of dispersion by the K electrons amount to $\Delta f'_R(\text{Co}) = -3.0$ and $f''_R(\text{Co}) = 3.4$, respectively (James, 1948).

† The inequality sign $>$ or $<$ shows that the observed intensity for (hkl) is larger or smaller than that for $(hk\bar{i}\bar{l})$. The sign $?>$ or $?<$ means that the inequality is not so definite as that without the symbol $?$. The symbol $?$ shows that the inequality between $I(hkil)$ and $I(hk\bar{i}\bar{l})$ could not be observed or was different according to different observers.

a complex ion $[\text{Co}(\text{en})_3]^{3+}$ shown in Fig. 1 corresponds to the dextrorotatory form with respect to the Na D line.

We wish to express our sincere thanks to Profs. I. Nitta and T. Watanabé for their kind advice and encouragement throughout this work. Part of the cost of this study was defrayed from the Scientific Research Grant of the Ministry of Education.

References

- BIJVOET, J. M., PEERDEMAN, A. F. & BOMMEL, A. J. VAN (1951). *Nature, Lond.* **168**, 271.
 JAMES, R. W. (1948). *The Optical Principles of the Diffraction of X-rays*, p. 609. London: Bell.
 SHIRO, M., NAKATSU, K., SAITO, Y. & KUROYA, H. (1955). To be published.