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THE CRYSTAL STRUCTURE OF $RbCoCl_3.2H_2O$

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EXPERIMENTAL

In view of the magnetic properties of $RbCoCl_3.2H_2O$ (1), it was considered worthwhile to determine the crystal structure, as the compound is not isomorphous with related compounds (2, 3, 4, 5). Crystals* of the title compound were studied on a four circle X-ray single-crystal diffractometer. The cell constants are a=15.714(6)Å, b=5.619(2)Å, c=8.743(3)Å and β=118.37(5)°. The space group is Cc or C2/c with four molecules in the unit cell. Intensities were measured with MoKα radiation (graphite monochromator) using the θ-2θ scanning technique. No absorption or extinction corrections were applied. The structure determination is based on 895 reflections, with a net intensity greater than twice the standard deviation based on counting statistics. An intensity distribution test (6) indicated a center of symmetry. Therefore the space group C2/c was assumed. As the number of equivalent positions in this space group is 8 the Rb, Co and at least one Cl atom have to be at special positions.

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RESULTS

Comparison of bond lengths in related compounds lead us to assume that the Rb, Co, and one of the Cl ions are at the special positions designated c, a and e in the International Tables for X-ray Crystallography (7). The y parameter of the Cl ion was chosen so as to give a reasonable Co-Cl distance. The remaining atoms were found from a difference Fourier-synthesis. Structural parameters (position and anisotropic temperature factors) were refined by the method of least-squares. Final positional parameters are given in Table 1.

TABLE 1
Final Positional Parameters of the Different Atoms

	x	y	z
Co	.0000	.0000	.0000
Cl1	.0000	.2065(5)	.2500
Cl2	.1434(2)	.2396(5)	.0529(4)
O	.0908(6)	-.2628(14)	.1607(10)
Rb	.2500	.2500	.0000

The resulting R-factor was 8.9%. In view of the absence of an absorption correction and the resulting high value of the R-factor, not much relevance can be assigned to the anisotropic temperature factors.

The structure consists of layers of Rb ions parallel to the bc plane. These layers alternate with layers containing octahedrally coordinated Co ions. The octahedra form infinite chains by sharing corners as indicated in Figure 1.

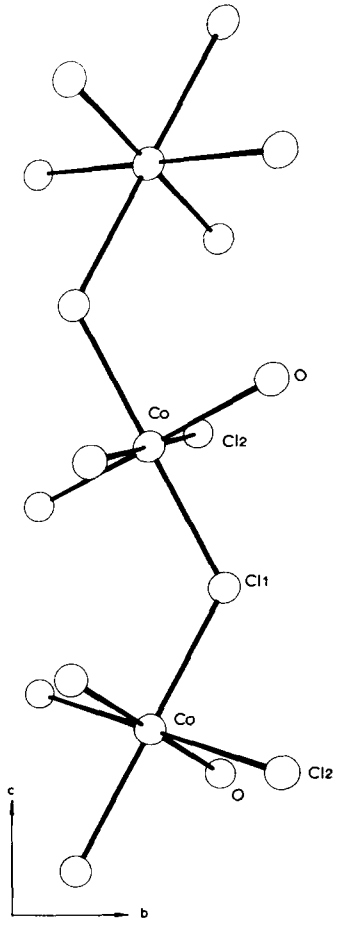

FIG. 1

Three dimensional representation showing the way in which the coordination octahedra are linked

As the Co ion is at a center of symmetry the water molecules have to occupy *trans*-positions. Bond distances found in the octahedra are Co-Cl1: 2.475(3)Å; Co-Cl2: 2.473(4)Å; Co-O: 2.070(8)Å. The values are in the range normally found for coordinated Co ions (3, 4). As far as bond angles are concerned the octahedra are quite regular. The angles found are Cl1-Co-Cl2: 87.8(2)°; Cl1-Co-O: 91.4(3)°; Cl2-Co-O: 89.3(4)°. It should be noted that the errors

quoted are, as usual, those given by the least squares procedure. Due to the absence of an absorption correction the error margins can increase significantly.

REFERENCES

1. J. FLOKSTRA, G.J. GERRITSMA, B. VAN DEN BRANDT and L.C. VAN DER MAREL, Phys. Lett., 53A, 159 (1975).
2. S.J. JENSEN, Acta Chem. Scand. 21, 889 (1967).
3. N. THORUP and H. SOLING, Acta Chem Scand. 23, 2933 (1969).
4. D.B. LOSEE, J.N. McELEARNY, J.E. SHANKLE, R.L. CARLIN, P.J. CRESSWELL and W.T. ROBINSON, Phys. Rev. B8, 2185 (1973).
5. J.W. METSELAAR and D. DE KLERK, Physica, 69, 499 (1973).
6. E.R. HOWELLS, D.C. PHILIPS and D. ROGERS, Acta Cryst. 3, 310 (1950).
7. International Tables for X-ray Crystallography, Vol. 1, (1962). Birmingham, Kynoch Press.