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The crystal structure of $MgClBr.6H_2O$.

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The crystal structure of $MgClBr.6H_2O$ is isomorphous with that of $MgCl_2.6H_2O$. Br and Cl atoms occupy at random the Cl sites in the latter structure.

Introduction

The crystal structures of $MgCl_2 . 6H_2O$ and $MgBr . 6H_2O$ were determined by Andress & Gundermann (1934). The structures are isomorphous; there are two molecules per unit cell and the space group is $C2/m$.

The material examined in this work was prepared by evaporating to dryness a solution containing 50% by molecular weight of each hexahydrate. The unit-cell dimensions of the resulting compound were determined from powder data obtained with Cu $K\alpha$ radiation using a de Wolff–Guinier camera, and are compared in Table 1 with the cell data given by Andress & Gundermann for $MgCl_2 . 6H_2O$ and $MgBr_2 . 6H_2O$.

Table 1. *Unit-cell data*

	a	b	c	β
$MgClBr.6H_2O$	$10{\cdot}05_3$ Å	$7{\cdot}24_3$ Å	$6{\cdot}16_0$ Å	93·85°
$MgCl_2.6H_2O$	9·90	7·15	6·10	94
$MgBr_2.6H_2O$	10·25	7·40	6·30	93·5

Structural analysis

Intensity data were obtained from c-axis equi-inclination Weissenberg multiple-film photographs of layer lines 0 to 3. The systematically absent reflexions were consistent with the space groups $C2/m$ and Cm. The intensities were measured using a Joyce–Loebl flying spot microdensitometer, visual estimates being made for weak reflexions. The data were then corrected for the Lorentz–polarization factor, for spot shape on upper layer lines (Phillips, 1954) and for absorption, assuming the crystal to be cylindrical in shape and using the appropriate factors given by Bond (1959).

In the structure of $MgCl_2 . 6H_2O$ and $MgBr_2 . 6H_2O$, Mg atoms are located at equipoint 2(*a*), halogen atoms at 4(*i*) and H_2O at 4(*i*) and 8(*j*). Assuming the structure of $MgClBr . 6H_2O$ to be similar, there are then two possibilities. Either Br and Cl atoms are distributed randomly at 4(*i*) in the centrosymmetric space group $C2/m$, or they are in ordered sites each at 2(*a*) in the space group Cm. Using as initial atomic coordinates those found by Andress & Gundermann for $MgCl_2 . 6H_2O$, and assuming an overall temperature factor of 2·5 Å^2, the random arrangement gave an R value of 15% and the ordered one 16% for $hk0$ and $hk1$ data. A three-dimensional least-squares refinement (Daly, Stephens & Wheatley, 1963) using the same intensity data reduced R to 11% for the random distribution, but hardly altered R for the ordered arrangement. At this stage it was concluded that the centrosymmetrical structure was the correct one. An electron density projection along the c-axis showed all the halogen peaks to be the same height, thereby confirming the proposed structure. A least-squares refinement using all the available intensity data gave $R=$ 13% for 275 reflexions. The final atomic parameters are listed in Table 2 with those found by Andress & Gundermann.

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Table 2. *Atomic parameters*

		x	y	z	B
$MgClBr.6H_2O$	Mg	0	0	0	2·40 (17) Å^2
	Cl, Br	0·3185 (3)	0	0·5211 (8)	2·87 (6)
	$H_2O(1)$	0·2025 (17)	0	0·1027 (44)	4·82 (39)
	$H_2O(2)$	−0·0428 (11)	0·2047 (17)	0·2135 (30)	4·56 (25)
$MgCl_2.6H_2O$	Mg	0	0	0	—
	Cl	0·318	0	0·615	—
	$H_2O(1)$	0·20	0	0·11	—
	$H_2O(2)$	−0·04	0·20	0·23	—

* In the structure of $MgBr_2.6H_2O$, x for Br = 0·320 and all other coordinates are the same as those for the $MgCl_2.6H_2O$ structure.