Octahedra link together by sharing edges to form α-PbO_2-like chains (Wells, 1985) that run parallel to *x*. Two SeO_3 groups link by sharing a corner to form an Se_2O_5 group, and the octahedral chains share corners with the Se_2O_5 groups to complete the structure. This is illustrated in Fig. 1, which shows the staggered octahedral chains viewed end-on and forming a centred array, with the Se_2O_5 groups linking the chains along both *y* and *z*.

Table 3 summarizes bond lengths and angles in selenite groups from fairly precisely determined inorganic crystal structures. The grand mean Se—O distance is 1·709 Å with a root-mean-square deviation of 0·010 Å, and the grand mean O—Se—O angle is 100·2° with a root-mean-square deviation of 1·3°.

There is significant variation of individual Se—O distances in the structures listed in Table 3. In previous work, this has been tacitly assumed to be in accord with bond-strength arguments. H-atom positions have been assigned on qualitative considerations of relative bond lengths, and Valkonen & Leskelä (1978) have reviewed Se—O and Se—OH distances in acid selenites, showing that Se—O and Se—OH distances cluster around 1·66 and 1·75 Å respectively. In order to put such arguments on a more quantitative basis, we have derived bond-valence curve parameters for the Se—O bond using selected data from Table 3 and fitting them to a curve of the general form $S = (R/R_0)^{-N}$ (Brown, 1981); the relevant parameters are $R_0 = 1{\cdot}808$ and $N = 5{\cdot}2$. This curve should help in deciphering hydrogen-bonding schemes, particularly in the more hydrated of the selenium oxysalts.

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Structure of Cadmium Dimagnesium Hexabromide Dodecahydrate, $CdMg_2Br_6.12H_2O$

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Abstract. $[Mg(H_2O)_6]_2[CdBr_6]$, $M_r = 856{\cdot}66$, rhombohedral, hexagonal setting, $R\bar{3}$ {Hall symbol $R\bar{3}$ [Hall (1981). *Acta Cryst.* A**37**, 517–525]}, $a = 10{\cdot}371\ (2)$, $c = 17{\cdot}761\ (2)$ Å, $V = 1654{\cdot}4$ Å^3, $Z = 3$, $D_x = 2{\cdot}58$ Mg m^{-3}, Mo *Kα* radiation, $\lambda = 0{\cdot}71069$ Å, $\mu = 11{\cdot}66$ mm^{-1}, $F(000) = 1206$, room temperature, $R = 0{\cdot}036$ ($wR = 0{\cdot}029$) for 1120 reflections. The sample was prepared from a saturated aqueous solution of $MgBr_2$ and $CdBr_2$ in a molar ratio of 2:1. The structure, which is the same as $[Mg(H_2O)_6]_2[CaCl_6]$, consists of two $Mg(H_2O)_6^{2+}$ (av. Mg—O = 2·055 Å) and one $CdBr_6^{4-}$ (Cd—Br = 2·788 Å) octahedral complexes linked by hydrogen bonds.

Introduction. Balarew, Duhlev & Panaiotov (1982) first reported the existence of the double salt $CdMg_2Br_6.12H_2O$ in the system $CdBr_2$–$MgBr_2$–H_2O at 298 K. This compound was subsequently predicted (Duhlev, 1984; Duhlev & Balarew, 1987) to possess a structure $[Mg(H_2O)_6]_2[CdBr_6]$ similar to $[Mg(H_2O)_6]_2[CaCl_6]$ (Leclaire, Borel & Monier, 1980; Clark, Evans & Erd, 1980), $[Mg(H_2O)_6]_2[CdCl_6]$ (Ledésert & Monier, 1981), and $[Ni(H_2O)_6]_2[CdCl_6]$ (Leclaire & Borel, 1982), where in each case the harder ligand, H_2O, is bonded to the harder cation and the softer one, the

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halogen ion, to the softer cation (Balarew & Duhlev, 1984). Although all these compounds contain the same structural motifs, $[M(H_2O)_6]_2[M'Cl_6]$, they belong to related but different space groups: $R\bar{3}$, $P31c$ and $P3$ respectively. The space group $R\bar{3}$ found for $[Mg(H_2O)_6]_2[CdBr_6]$ suggested that it would be isostructural with $[Mg(H_2O)_6]_2[CaCl_6]$ and this was confirmed by the analysis.

Experimental. A cylindrical, colourless hygroscopic crystal with diameter 0·16 mm and length 0·35 mm was sealed in a thin-walled capillary under dry nitrogen and mounted on a Syntex $P2_1$ diffractometer. Unit-cell parameters were determined from 15 well centred reflections in the range $20 < 2\theta < 30°$. The intensities were measured using a C-centred monoclinic cell but were transformed into the hexagonal cell for refinement. No correction was made for absorption since application of a ψ-scan absorption correction made no difference to either the refined parameters or the agreement index even though the maximum correction factor was 1·40 (reflection 310). Intensities were measured for 1120 reflections with $0 \leq h \leq 21$, $-3 \leq k \leq 12$, $-10 \leq l \leq 7$ (hexagonal setting) and $2\theta < 50°$. The $9\bar{3}\bar{3}$ and 332 reflections were used as standards and they varied by less than 1·8%. Equivalent reflections were averaged ($R_{\rm int} = 0·017$) to give 657 unique reflections. The heavy-atom coordinates for the isostructural $[Mg(H_2O)_6]_2[CaCl_6]$ (Clark *et al.*, 1980) were used as the initial model. The positions of the H atoms were found using the difference map. A weight $w = [\sigma^2(F_o) + kF_o^2]^{-1}$ was used where k refined to 0·000249 and $\sigma(F_o)$ is the error derived from counting statistics. The scale factor, weighting factor (k), extinction coefficient and all variable positional and atomic displacement parameters were refined by least squares [function minimized $= \sum w(|F_o| - |F_c|)^2$] using *SHELX*76 (Sheldrick, 1976). The final agreement indices based on the use of all non-equivalent reflections are $R = 0·036$ and $wR = 0·029$ and the goodness of fit $S = 1·08$ [$R = 0·027$, $wR = 0·024$ and $S = 1·17$ when 107 reflections with $F < 3\sigma(F)$ were omitted]. The average shift/e.s.d. = 0·007 (max. = 0·015). The final difference electron density has maximum and minimum values of +0·65 and −0·43 e Å^{-3} respectively. The secondary-extinction coefficient (Larson, 1967) $g = 0·00045$ (4). Complex atomic scattering factors for neutral atoms were taken from *International Tables for X-ray Crystallography* (1974). The final atomic coordinates and temperature factors are given in Table 1.*

Discussion. The bond distances and angles are shown in Table 2. In agreement with the prediction (Duhlev, 1984; Duhlev & Balarew, 1987), the structure is built up of two kinds of independent complex ions, $Mg(H_2O)_6^{2+}$ and $CdBr_6^{4-}$, in the ratio 2:1. Both are, within

Table 1. *Atomic positions and equivalent isotropic atomic displacement factors* (Å²)

$U_{\rm eq} = \frac{1}{3}(U_{11} + U_{22} + U_{33})$ or $U_{\rm iso}$ (for H atoms).

	x	y	z	$U_{\rm eq}$
Cd	0	0	0	0·0347
Mg	0	0	0·32520 (13)	0·0470
Br	0·16964 (5)	−0·07548 (5)	0·09234 (3)	0·0440
O(1)	0·1851 (4)	0·0715 (5)	0·2586 (2)	0·0446
O(2)	−0·1864 (5)	−0·0663 (5)	0·3908 (2)	0·0537
H(11)	0·181 (9)	0·026 (9)	0·226 (4)	0·10 (3)
H(12)	0·267 (6)	0·167 (6)	0·261 (3)	0·07 (2)
H(21)	−0·207 (7)	−0·004 (9)	0·411 (3)	0·08 (2)
H(22)	−0·235 (7)	−0·141 (7)	0·395 (4)	0·07 (3)

Table 2. *Interatomic distances* (Å) *and angles* (°)

		O(1)–Mg–O(1)	90·1 (2)
Mg–O(1)	2·052 (4) (× 3)	O(1)–Mg–O(2)	90·5 (2)
Mg–O(2)	2·059 (4) (× 3)	O(1)–Mg–O(2)	88·2 (2)
		O(2)–Mg–O(2)	91·1 (2)
Cd–Br	2·7884 (7) (× 6)	Br–Cd–Br	88·86 (2)*
		Br–Cd–Br	91·02 (2)

O–H···Br	O–H	H···Br	O···Br	∠OHBr	∠HOH
O(1)–H(11)···Br	0·73 (8)	2·58 (8)	3·290 (4)	165·0 (9)	117·0 (6)
O(1)–H(12)···Br$^{\rm i}$	0·93 (5)	2·47 (4)	3·388 (3)	167·0 (5)	
O(2)–H(21)···Br$^{\rm ii}$	0·86 (10)	2·53 (10)	3·309 (6)	151·0 (5)	119·0 (8)
O(2)–H(22)···Br$^{\rm iii}$	0·69 (6)	2·85 (4)	3·432 (6)	144·0 (8)	

Symmetry code: (i) $\frac{2}{3}-x, \frac{1}{3}-y, \frac{1}{3}-z$; (ii) $-\frac{1}{3}+x, \frac{1}{3}+y, \frac{1}{3}+z$; (iii) $-\frac{1}{3}-y, \frac{2}{3}+x-y, \frac{1}{3}+z$.

* Angle between Br atoms related by the threefold axis.

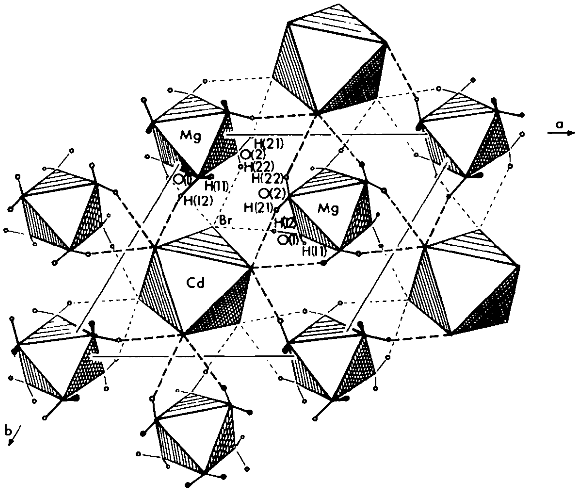

Fig. 1. The structure of the layer of $[Mg(H_2O)_6]_2[CdBr_6]$ at $z = \frac{2}{3}$ viewed down the c axis. The hydrogen bonds in the layer are shown. The H(11) atoms form hydrogen bonds (not shown) with the Br atoms belonging to the $CdBr_6$ octahedron above (or below) the respective $Mg(H_2O)_6$ octahedron.

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* Lists of structure factors and anisotropic atomic displacement factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44209 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

the accuracy of the experiment, undistorted octahedra. The ions are held together by O—H···Br hydrogen bonds. The structure is composed of linear $[Mg(H_2O)_6]^{2+}[CdBr_6]^{4-}[Mg(H_2O)_6]^{2+}$ triplets with the three metal atoms lying on the same threefold axis and each $Mg(H_2O)_6^{2+}$ ion forming three hydrogen bonds to the adjacent $CdBr_6^{4-}$ ion along the threefold axis. The remaining hydrogen bonds link the $CdBr_6^{4-}$ ion to its six $Mg(H_2O)_6^{2+}$ neighbours lying in the *ab* plane. A projection of the structure viewed down the *c* axis is shown in Fig. 1. The present structure differs from the trigonal ones in the arrangements of the ions along the threefold axis. In the rhombohedral structure each $Mg(H_2O)_6^{2+}$ ion has four CdX_6^{4-} neighbours. In the trigonal structures one $Mg(H_2O)_6^{2+}$ ion has three, the other five CdX_6^{4-} neighbours.

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Structure of Magnesium Dizinc Hexabromide Hexahydrate, $MgZn_2Br_6.6H_2O$

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Abstract. $[Mg(H_2O)_6][Zn_2Br_6]$, $M_r = 742{\cdot}59$, orthorhombic, *Immm* {Hall symbol $\bar{I}22$ [Hall (1981). *Acta Cryst.* A**37**, 517–525]}, $a = 10{\cdot}447(2)$, $b = 10{\cdot}325(1)$, $c = 7{\cdot}999(2)$ Å, $V = 862{\cdot}8$ Å^3, $Z = 2$, $D_x = 2{\cdot}86$ Mg m^{-3}, Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71069$ Å, $\mu = 16{\cdot}35$ mm^{-1}, $F(000) = 684$, room temperature, $R = 0{\cdot}057$ ($wR = 0{\cdot}056$) for 890 reflections. Prepared from a saturated aqueous solution of $MgBr_2$ and $ZnBr_2$ in a molar ratio of 1:2. The structure consists of independent octahedral $Mg(H_2O)_6^{2+}$ complexes (Mg—O = 2·04 Å) and dimeric tetrahedral $Zn_2Br_6^{2-}$ complexes [Zn—Br = 2·48 Å (bridging) and 2·36 Å (terminal)], linked together by H bonds.

Introduction. The title compound was first described by Duhlev & Balarew (1986) as one of the solid phases crystallizing in the ternary system $MgBr_2$–$ZnBr_2$–H_2O at 298 K. Using a method (Balarew & Duhlev, 1984) based on the relative softness of the ions (Pearson, 1963), Duhlev & Balarew (1986) predicted that the structure would contain independent $Mg(H_2O)_6$ octahedra and $ZnBr_4$ tetrahedra, the later sharing either corners to link into an infinite chain $(ZnBr_3)_\infty$ or edges to form discrete Zn_2Br_6 dimers.

Before the X-ray study was undertaken the structure was modelled using the cell reported by Brehler (1961) for the isostructural (Duhlev & Balarew, 1986) $ZnBr_2.2H_2O$ and the space group *Immm*. As a $(ZnBr_3)_\infty$ chain could not be fitted into this cell, the dimer was selected. With the aid of the program *STRUMO* (Brown, 1987) the model was refined to give atomic positions within 0·05 Å of those found.

Experimental. $MgZn_2Br_6.6H_2O$ forms colourless, extremely hygroscopic crystals. Therefore, a cylindrical crystal with diameter 0·2 mm and length 0·3 mm was sealed in a thin-walled capillary under dry nitrogen and mounted on a Nicolet *P*3 diffractometer. Unit-cell parameters were determined from 15 well centred strong reflections in the range $20 < 2\theta < 38°$. Empirical absorption corrections were derived from ψ-scans of 15 reflections (maximum correction factor of 1·70 for the intensity of reflection 222). Intensities were

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