

Se—O—H angles of 106 and 118° would result from these interactions. Both these hydrogen bonds also lead to short non-bonding Se to H distances of less than 2.4 Å.

This compound is the first layered anhydrous selenite to be discovered, complementing the layered praseodymium selenite/diselenite phase  $\text{PrH}_3(\text{SeO}_3)_2(\text{Se}_2\text{O}_5)$  (Koskenlinna & Valkonen, 1977), and layered hydrated selenite phases such as  $\text{CaSeO}_3 \cdot \text{H}_2\text{O}$  (Hawthorne, Ercit & Groat, 1986) and the recently discovered  $\text{LnHSe}_2\text{O}_6 \cdot 2\text{H}_2\text{O}$ , Ln = Y, Pr—Yb (except Pm) (Morris, Harrison, Srdanov, Stucky & Cheetham, 1991). The two-dimensional structure of  $\text{LaHSe}_2\text{O}_6$ , which is layered with respect to the polar crystallographic direction, combined with the acidic protons which must be present, leads to interesting possibilities for ion exchange and intercalation chemistry. Studies of these reactions are now being undertaken.

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#### References

- BAIRD, P. D. (1987). *RC85. Data Reduction Program*. Chemical Crystallography Laboratory, Univ. of Oxford, England.
- CARRUTHERS, J. R. & WATKIN, D. J. (1979). *Acta Cryst.* **A35**, 698–699.
- DELAGE, C., CARPY, A., H'NAÏFI, A. & GOURSELLE, M. (1986). *Acta Cryst.* **C42**, 1475–1477.
- HAWTHORNE, F. C., ERCIT, T. S. & GROAT, L. A. (1986). *Acta Cryst.* **C42**, 1285–1287.
- HAWTHORNE, F. C., GROAT, L. A. & ERCIT, T. S. (1987). *Acta Cryst.* **C43**, 2044–2046.
- KOSKENLINNA, M. & VALKONEN, J. (1977). *Acta Chem. Scand. Ser. A*, **31**, 457–460.
- LE PAGE, Y. (1988). *J. Appl. Cryst.* **21**, 983–984.
- MORRIS, R. E., HARRISON, W. T. A., SRDANOV, V. I., STUCKY, G. D. & CHEETHAM, A. K. (1991). In preparation.
- MORRIS, R. E., HRILJAC, J. A. & CHEETHAM, A. K. (1990). *Acta Cryst.* **C46**, 2013–2017.
- SHELDRICK, G. M. (1986). *SHELXS86. User's Guide*. Univ. of Göttingen, Germany.
- WASER, J. (1974). *Acta Cryst.* **A30**, 261–264.
- WATKIN, D. J., CARRUTHERS, J. R. & BETTERIDGE, P. W. (1986). *Crystals User's Guide*. Chemical Crystallography Laboratory, Univ. of Oxford, England.

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## The Structure of Hexaaquaaluminium(III) Bromate Trihydrate, [Al(H<sub>2</sub>O)<sub>6</sub>](BrO<sub>3</sub>)<sub>3</sub>·3H<sub>2</sub>O

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**Abstract.** Hexaaquaaluminium(III) bromate trihydrate,  $[\text{Al}(\text{H}_2\text{O})_6](\text{BrO}_3)_3 \cdot 3\text{H}_2\text{O}$ ,  $M_r = 572.84$ , triclinic,  $P\bar{1}$ ,  $a = 9.536$  (2),  $b = 11.095$  (4),  $c = 9.291$  (2) Å,  $\alpha = 106.58$  (2),  $\beta = 100.42$  (2),  $\gamma = 113.01$  (2)°,  $V = 818.1$  (4) Å<sup>3</sup>,  $Z = 2$ ,  $D_x = 2.33$  g cm<sup>-3</sup>,  $\lambda(\text{Mo } K\alpha) = 0.71073$  Å,  $\mu = 74.58$  cm<sup>-1</sup>,  $F(000) = 560$ ,  $T = 296$  K,  $R = 0.050$  for 3777 unique reflections having  $I > \sigma_I$ . The single type of Al ion is coordinated by six inequivalent water O atoms which form a slightly distorted octahedron. The average Al—O distance within the octahedron is 1.872 (11) Å. Each of the three inequivalent bromate groups has three inequivalent O atoms. The average Br—O distances and O—Br—O angles for these ions are: 1.652 (25) Å and 104.1 (17)° for Br(1)O<sub>3</sub>; 1.650 (9) Å and 104.4 (18)° for Br(2)O<sub>3</sub>; 1.643 (9) Å

and 103.6 (14)° for Br(3)O<sub>3</sub>. The aluminium–oxygen complex conformed to rigid-body behavior but the bromate groups did not. Corrected for rigid-body motion, the average Al—O distance becomes 1.880 (10) Å. Least-squares refinement of the positional parameters of the 18 inequivalent H atoms permitted a detailed analysis of the hydrogen bonding.

**Introduction.** Continuing interest in structures of simple hydrated oxyhalogen salts led to the present study of hydrated aluminium bromate. As in our previous studies, it was of particular interest to refine H-atom coordinates in order to carry out a detailed analysis of the hydrogen bonding.

**Experimental.** Metathetical reaction of aqueous solutions of  $\text{Al}_2(\text{SO}_4)_3$  (Aldrich Chemical Company) and

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Ba(BrO<sub>3</sub>)<sub>2</sub> (Strem Chemicals) in very nearly stoichiometric proportion followed by removal of BaSO<sub>4</sub> by filtration produced a dilute Al(BrO<sub>3</sub>)<sub>3</sub> solution. Evaporation over concentrated H<sub>2</sub>SO<sub>4</sub> at approximately 285 K produced a cloudy crystalline mass. Recrystallization at room temperature produced the experimental sample, a clear colorless chunk with approximate principal dimensions 0.23 × 0.31 × 0.38 mm. The sample was coated with a thin layer of Apiezon L grease to retard potential loss or gain of water and was analyzed at 296 K with a Rigaku AFC5S diffractometer utilizing graphite-monochromated Mo K $\alpha$  radiation.

Unit-cell parameters were obtained from a least-squares fit of the setting angles for 25 centered reflections with 28 < 2 $\theta$  < 30°. Intensity data were measured for 6228 reflections (exclusive of standards) with +*h*,  $\pm k$ ,  $\pm l$  indices ( $h_{\max} = 14$ ,  $k = -16$  to 16,  $l = -14$  to 14) and with 2 $\theta$  in the range 4  $\leq$  2 $\theta$   $\leq$  65°. The  $\omega$ -2 $\theta$  scan technique was employed with scan widths (1.20 + 0.35tan $\theta$ )° in  $\omega$ , and a background/scan time-ratio of 0.5. A variance was assigned to each reflection by means of the formula  $\sigma_I^2 = \sigma_{cs}^2(I) + (0.03I)^2$ , in which  $\sigma_{cs}$  is based on counting statistics and *I* is the integrated intensity. Six standard reflections (1 $\bar{1}\bar{1}$ , 2 $\bar{1}\bar{1}$ , 102, 3 $\bar{8}\bar{2}$ , 323 and 2 $\bar{4}\bar{6}$ ) were measured after every 150 reflections and exhibited, on average, a maximum relative intensity variation of  $\pm 6.3\%$ . The first three standards listed above can be categorized as low-angle standards (2 $\theta$  < 13°). These standards displayed intensity growth, primarily in the later stages of data collection. The high-angle standards (2 $\theta$  > 29°), the remaining three, were stable throughout the data collection: they exhibited, on average, a maximum non-systematic relative intensity variation of  $\pm 2.3\%$ . Since the low-angle data had been collected before the low-angle standards began displaying growth and since the high-angle standards were quite stable, no growth correction was made. The data were corrected for Lorentz and polarization effects.  $\psi$ -scan data were obtained just after the 30° shell intensity data were collected; the range of transmission factors was 0.442–1.000, with an average value of 0.777.

The intensity data were found to belong to Laue group  $\bar{1}$ ; of the two allowed space groups, the centrosymmetric alternative  $P\bar{1}$  (No. 2) was given initial preference. Since refinement proceeded well, this space group was adopted. The direct-methods program *SHELXS86* (Sheldrick, 1985) gave initial positions for Br(1), Br(2), Br(3) and Al atoms. Fourier difference methods were then used to locate the remaining O and H atoms. All atoms were assigned to general positions. Full-matrix least-squares refinement was performed using the *TEXSAN* structure analysis package (Molecular Structure Corporation, 1989) to minimize the func-

tion  $\sum \sigma_F^{-2}(|F_o| - |F_c|)^2$  in which  $\sigma_F = \sigma_I/2FLp$ . Neutral-atom scattering factors and anomalous-dispersion factors were taken from Cromer & Waber (1974) for Al, Br and O; the scattering factor for H was taken from Stewart, Davidson & Simpson (1965).

Following isotropic refinement of all the non-H atoms, the  $\psi$ -scan absorption correction was applied and all symmetry-equivalent reflections were averaged ( $R_{\text{int}} = 0.040$  for 309 doublets). The secondary-extinction coefficient (Zachariasen, 1963, 1968) was treated as an adjustable parameter and the refinement proceeded to the anisotropic stage for all atoms except H and to the isotropic stage for H. Atoms H(6), H(17) and H(18) could not be located using a Fourier difference map until only reflections with 2 $\theta$  < 40° were used to generate the map. After all atoms had been located, refinement proceeded using all data with  $I > \sigma_I$ .

The results for the final refinement cycle were: 3777 independent observations with  $I > \sigma_I$ , 272 variables;  $R = 0.050$ ;  $wR = 0.047$ ;  $w = \sigma_F^{-2}$ ;  $S = 1.38$ ;  $(\Delta/\sigma)_{\max} = 0.01$ . The final refined value of the secondary-extinction coefficient was 1.28 (2)  $\times 10^{-5}$ ; the largest correction for secondary extinction was 57% for the 12 $\bar{1}$  reflection. The maximum peak in the final electron density difference map was +1.1 e  $\text{\AA}^{-3}$  in value and was located near (0.93, 0.67, 0.70),  $\sim 0.8$   $\text{\AA}$  from O(22) and 0.9  $\text{\AA}$  from Br(2); the minimum peak was  $-1.0$  e  $\text{\AA}^{-3}$  in value and was located near (0.93, 0.02, 0.41),  $\sim 0.8$   $\text{\AA}$  from Br(3).

The final atomic coordinates and isotropic and equivalent isotropic displacement parameters and their e.s.d.'s are given in Table 1.\* Selected interatomic distances and angles in the coordination polyhedron about Al, in the bromate ions and in the water molecules are given in Table 2 together with their uncertainties. Hydrogen bonds are tabulated in Table 3 (deposited) and are discussed below. A unit cell for this structure is shown in Fig. 1.

Rigid-body analysis was performed using the program *THMA11* (Trueblood, 1986), based on the work of Schomaker & Trueblood (1968). The average magnitude of the differences in the mean-square displacement amplitudes (m.s.d.a.) along the interatomic vectors for the 21 unique atom pairs of the aluminium–oxygen complex was found to be 34 (32)  $\times 10^{-4}$   $\text{\AA}^2$ . Thus, Hirshfeld's (1976) rigid-bond test,

\* Lists of structure factors and anisotropic displacement parameters and supplementary material relating to the rigid-body analysis and the hydrogen bonding have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54960 (44 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR0351]

Table 1. *Final positional parameters and equivalent isotropic and isotropic displacement parameters for hexaquaaluminium bromate trihydrate at 296 K*

E.s.d.'s are in parentheses.  
 $B_{eq} = (8\pi^2/3)\sum_i U_{ij} a_i^* a_j^* a_i \cdot a_j$

	x	y	z	$B_{eq}/B (\text{\AA}^2)$
Br(1)	0.25065 (7)	0.68199 (6)	0.09851 (6)	1.90 (2)
Br(2)	0.99724 (7)	0.62526 (6)	0.68541 (6)	1.63 (1)
Br(3)	0.87096 (7)	0.00804 (6)	0.32202 (6)	1.95 (2)
Al	0.43311 (20)	0.18053 (16)	0.30032 (17)	1.44 (4)
O(1)	0.5214 (6)	0.3016 (5)	0.1993 (5)	2.0 (1)
O(2)	0.3495 (6)	0.2974 (5)	0.3949 (5)	2.2 (1)
O(3)	0.2410 (5)	0.0750 (5)	0.1270 (5)	2.1 (1)
O(4)	0.3488 (5)	0.0552 (5)	0.3980 (5)	2.0 (1)
O(5)	0.5164 (7)	0.0634 (5)	0.2002 (6)	2.4 (1)
O(6)	0.6214 (6)	0.2863 (5)	0.4749 (5)	2.4 (1)
O(11)	0.3173 (5)	0.7850 (4)	0.0001 (4)	2.6 (1)
O(12)	0.3406 (7)	0.5837 (5)	0.0755 (5)	3.7 (2)
O(13)	0.3399 (6)	0.7979 (4)	0.2874 (4)	2.7 (1)
O(21)	0.9703 (5)	0.5198 (4)	0.7822 (5)	2.7 (1)
O(22)	0.9351 (5)	0.7387 (4)	0.7687 (5)	2.7 (1)
O(23)	0.8564 (5)	0.5283 (4)	0.5073 (4)	2.5 (1)
O(31)	0.8145 (6)	-0.1030 (5)	0.4117 (5)	3.2 (1)
O(32)	0.8481 (7)	0.1425 (5)	0.4235 (6)	4.0 (2)
O(33)	0.7240 (6)	-0.0651 (7)	0.1527 (5)	5.3 (2)
O(41)	0.4143 (7)	0.4279 (5)	0.7156 (5)	2.8 (1)
O(42)	0.0988 (9)	0.3234 (7)	0.7374 (7)	4.2 (2)
O(43)	0.9946 (8)	0.1626 (6)	0.9048 (7)	4.4 (2)
H(1)	0.523 (9)	0.394 (9)	0.214 (9)	5.1 (19)†
H(2)	0.548 (10)	0.280 (8)	0.152 (9)	3.6 (22)†
H(3)	0.250 (8)	0.297 (6)	0.342 (7)	2.4 (13)†
H(4)	0.351 (7)	0.329 (6)	0.471 (7)	1.3 (13)†
H(5)	0.167 (9)	0.000 (7)	0.118 (8)	3.2 (17)†
H(6)	0.242 (11)	0.084 (9)	0.047 (10)	6.1 (24)†
H(7)	0.298 (8)	0.061 (6)	0.467 (7)	2.7 (14)†
H(8)	0.347 (8)	-0.022 (7)	0.372 (8)	3.1 (16)†
H(9)	0.470 (7)	-0.008 (6)	0.150 (7)	1.0 (13)†
H(10)	0.613 (12)	0.053 (10)	0.242 (11)	8.6 (29)†
H(11)	0.721 (12)	0.390 (10)	0.501 (10)	8.4 (27)†
H(12)	0.616 (11)	0.268 (9)	0.536 (9)	5.4 (25)†
H(13)	0.331 (9)	0.393 (8)	0.730 (8)	3.6 (19)†
H(14)	0.498 (9)	0.413 (7)	0.785 (8)	3.5 (16)†
H(15)	0.032 (10)	0.263 (8)	0.635 (9)	5.0 (21)†
H(16)	0.075 (10)	0.368 (8)	0.756 (9)	2.6 (20)†
H(17)	1.027 (10)	0.212 (8)	0.856 (9)	5.1 (22)†
H(18)	1.016 (12)	0.193 (10)	0.977 (10)	5.3 (28)†

† Refined isotropically; coordinates as observed (not neutron adjusted).

extended as described by Rosenfield, Trueblood & Dunitz (1978), is satisfied for the aluminium-oxygen complex. Corrections for the rigid-body motion have been applied and the corrected Al—O bond lengths tabulated in Table 2. None of the three independent bromate groups was found to conform to the rigid-body model.

**Discussion.** The single Al cation is coordinated by six water molecules to form a slightly distorted octahedron. The average observed Al—O distance is 1.872 (11) Å and no angle departs by more than 2.3° from the corresponding angle in a regular octahedron. Previously reported Al—O distances in hexaquaaluminium complexes in nine selected salts range from 1.843 to 1.923 Å with an average value of 1.883 (18) Å (Buchanan & Harris, 1968; Cradwick & de Endredy, 1975, 1977; Cromer, Kay & Larson, 1966; Larson & Cromer, 1967; Punte, Rivero & Rigotti, 1987; Schein, Lingafelter & Stewart, 1967). Corrected for rigid-body motion, the average Al—O distance in the present salt becomes 1.880 (10) Å.

Table 2. *Selected bond distances (Å) and angles (°) for hexaquaaluminium bromate trihydrate*

E.s.d.'s are in parentheses.

Coordination polyhedron	Observed distance	Rigid-body distance		
Al—O(1)	1.874 (5)	1.880	O(1)—Al—O(2)	90.3 (2)
Al—O(2)	1.871 (4)	1.879	O(1)—Al—O(3)	90.3 (2)
Al—O(3)	1.871 (4)	1.880	O(1)—Al—O(4)	177.7 (2)
Al—O(4)	1.874 (4)	1.880	O(1)—Al—O(5)	88.5 (2)
Al—O(5)	1.889 (5)	1.897	O(1)—Al—O(6)	90.2 (2)
Al—O(6)	1.856 (5)	1.865	O(2)—Al—O(3)	89.4 (2)
O(1)—O(2)	2.657 (6)	2.666	O(2)—Al—O(4)	92.0 (2)
O(1)—O(3)	2.656 (7)	2.666	O(2)—Al—O(5)	178.6 (2)
O(1)—O(4)	3.748 (6)	3.759	O(2)—Al—O(6)	89.6 (2)
O(1)—O(5)	2.626 (6)	2.634	O(3)—Al—O(4)	89.9 (2)
O(1)—O(6)	2.643 (6)	2.653	O(3)—Al—O(5)	89.8 (2)
O(2)—O(3)	2.631 (6)	2.641	O(3)—Al—O(6)	178.8 (2)
O(2)—O(4)	2.694 (6)	2.702	O(4)—Al—O(5)	89.2 (2)
O(2)—O(5)	3.760 (6)	3.775	O(4)—Al—O(6)	89.6 (2)
O(2)—O(6)	2.627 (7)	2.639	O(5)—Al—O(6)	91.3 (2)
O(3)—O(4)	2.646 (6)	2.656		
O(3)—O(5)	2.654 (7)	2.668		
O(3)—O(6)	3.727 (6)	3.744		
O(4)—O(5)	2.643 (6)	2.652		
O(4)—O(6)	2.629 (6)	2.639		
O(5)—O(6)	2.677 (7)	2.688		
<b>Bromate groups</b>				
Br(1)—O(11)	1.669 (4)		O(11)—Br(1)—O(12)	104.2 (2)
Br(1)—O(12)	1.623 (5)		O(11)—Br(1)—O(13)	102.3 (2)
Br(1)—O(13)	1.665 (4)		O(12)—Br(1)—O(13)	105.7 (2)
Br(2)—O(21)	1.641 (4)		O(21)—Br(2)—O(22)	105.0 (2)
Br(2)—O(22)	1.652 (4)		O(21)—Br(2)—O(23)	105.8 (2)
Br(2)—O(23)	1.658 (4)		O(22)—Br(2)—O(23)	102.3 (2)
Br(3)—O(31)	1.653 (4)		O(31)—Br(3)—O(32)	103.3 (2)
Br(3)—O(32)	1.639 (4)		O(31)—Br(3)—O(33)	105.1 (3)
Br(3)—O(33)	1.637 (5)		O(32)—Br(3)—O(33)	102.4 (3)
<b>Water molecules</b>				
O(1)—H(1)	0.99 (8)		H(1)—O(1)—O(2)	117 (8)
O(1)—H(2)	0.58 (7)			
O(2)—H(3)	0.99 (7)		H(3)—O(2)—H(4)	94 (6)
O(2)—H(4)	0.69 (5)			
O(3)—H(5)	0.83 (7)		H(5)—O(3)—H(6)	114 (7)
O(3)—H(6)	0.77 (8)			
O(4)—H(7)	0.87 (6)		H(7)—O(4)—H(8)	109 (6)
O(4)—H(8)	0.82 (7)			
O(5)—H(9)	0.70 (5)		H(9)—O(5)—H(10)	94 (7)
O(5)—H(10)	1.00 (10)			
O(6)—H(11)	1.09 (10)		H(11)—O(6)—H(12)	116 (8)
O(6)—H(12)	0.66 (7)			
O(41)—H(13)	0.79 (7)		H(13)—O(41)—H(14)	109 (6)
O(41)—H(14)	1.02 (7)			
O(42)—H(15)	0.92 (8)		H(15)—O(42)—H(16)	105 (9)
O(42)—H(16)	0.61 (7)			
O(43)—H(17)	0.81 (7)		H(17)—O(43)—H(18)	117 (10)
O(43)—H(18)	0.61 (8)			

Each of three inequivalent bromate ions in the structure has three inequivalent O atoms. The average observed Br—O distances and O—Br—O angles for these three ions are: 1.652 (25) Å and 104.1 (17)° for Br(1)O<sub>3</sub>; 1.650 (9) Å and 104.4 (18)° for Br(2)O<sub>3</sub>; 1.643 (9) Å and 103.6 (14)° for Br(3)O<sub>3</sub>. These values are in good agreement with those reported previously from this laboratory for bromate ions (Blackburn, Gallucci & Gerkin, 1990, 1991).

Nine inequivalent water-molecule O atoms are present in this structure. Of these, six are coordinated to Al, two are coordinated to two H atoms and one is coordinated to a single H atom. Each water molecule was assigned to a hydrate class (Ferraris & Franchini-Angela, 1972): water molecules containing O(1) through O(6) belong to

hydrate class *M*, O(41) and O(42) belong to hydrate class *E*, and O(43) belongs to hydrate class *F*. Each H-atom position was altered along the direction of the corresponding O—H bond as determined by X-ray diffraction until the O—H distance matched the average distance for that particular hydrate class as determined by neutron diffraction (0.967 Å for class *M*; 0.966 Å for class *E*; 0.948 Å for class *F*) (Chiari & Ferraris, 1982). This was done to account for the usual foreshortening of the O—H bond as determined by X-ray diffraction. In the present study, however, five of the 18 O—H bond lengths as determined by X-ray diffraction are longer than the average values given by neutron diffraction. For consistency, however, these five proton positions were also neutron adjusted. The neutron-adjusted H...O(acceptor) distance is shorter than the observed distance in all but these five cases. The neutron-adjusted H...O(acceptor) distances will be taken as the hydrogen-bond lengths. Our analysis of hydrogen bonding is based partially on the work of Jeffrey (1987) and Chiari & Ferraris (1982).

Excluding bifurcated hydrogen bonds, the average hydrogen-bond length is 1.87 (24) Å and the average O—H...O angle is 161 (23)°. There are four cases of two-centered/bifurcated hydrogen bonding. The average bifurcated hydrogen-bond length is 2.77 (31) Å and the corresponding average O—H...O angle is 111 (17)°.

Each water molecule donates two hydrogen bonds with H...O(acceptor) distances of less than 2.00 Å except for the O(5) water molecule, which donates

only one within this distance. That same water molecule is, however, involved in the strongest of the four bifurcated hydrogen bonds. Each bromate O atom acts as an acceptor for at least one hydrogen bond, while the average number of hydrogen bonds involving each bromate O atom is greater than two. Thus a complex three-dimensional network of hydrogen bonds extends throughout the structure.

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#### References

- BLACKBURN, A. C., GALLUCCI, J. C. & GERKIN, R. E. (1990). *Acta Cryst.* **B46**, 712–716.
- BLACKBURN, A. C., GALLUCCI, J. C. & GERKIN, R. E. (1991). *Acta Cryst.* **C47**, 1786–1789, 2019–2023.
- BUCHANAN, D. R. & HARRIS, P. M. (1968). *Acta Cryst.* **B24**, 954–960.
- CHIARI, G. & FERRARIS, G. (1982). *Acta Cryst.* **B38**, 2331–2341.
- CRADWICK, P. D. & DE ENDREDEY, A. S. (1975). *J. Chem. Soc. Dalton Trans.* pp. 1926–1929.
- CRADWICK, P. D. & DE ENDREDEY, A. S. (1977). *J. Chem. Soc. Dalton Trans.* pp. 146–149.
- CROMER, D. T., KAY, M. I. & LARSON, A. C. (1966). *Acta Cryst.* **21**, 383–389.
- CROMER, D. T. & WABER, J. T. (1974). In *International Tables for X-ray Crystallography*, Vol. IV, pp. 71, 148. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
- FERRARIS, G. & FRANCHINI-ANGELA, M. (1972). *Acta Cryst.* **B28**, 3572–3583.
- HIRSHFELD, F. L. (1976). *Acta Cryst.* **A32**, 239–244.
- JEFFREY, G. A. (1987). *The Nanometer World of Hydrogen Bonds*. In *Patterson and Pattersons*, edited by J. P. GLUSKER, B. K. PATTERSON & M. ROSSI, pp. 193–221. Oxford Univ. Press.
- JOHNSON, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, TN, USA.
- LARSON, A. C. & CROMER, D. T. (1967). *Acta Cryst.* **22**, 793–800.
- Molecular Structure Corporation. (1989). *TEXSAN. TEXRAY Structure Analysis Package*. Version 5.0. MSC, 3200A Research Forest Drive, The Woodlands, TX 77381, USA.
- PUNTE, G., RIVERO, B. E. & RIGOTTI, G. (1987). *Acta Cryst.* **C44**, 216–219.
- ROSENFELD, R. E., TRUEBLOOD, K. N. & DUNITZ, J. D. (1978). *Acta Cryst.* **A34**, 828–829.
- SCHEIN, B. J. B., LINGAFELTER, E. C. & STEWART, J. M. (1967). *J. Chem. Phys.* **47**, 5183–5189.
- SCHOMAKER, V. & TRUEBLOOD, K. N. (1968). *Acta Cryst.* **B24**, 63–76.
- SHELDRIK, G. M. (1985). In *Crystallographic Computing 3*, edited by G. M. SHELDRIK, C. KRUGER & R. GODDARD, pp. 175–189. Oxford Univ. Press.
- STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.
- TRUEBLOOD, K. N. (1986). *THMA11*. Univ. of California, Los Angeles, CA 90024, USA.
- ZACHARIASEN, W. H. (1963). *Acta Cryst.* **16**, 1139–1144.
- ZACHARIASEN, W. H. (1968). *Acta Cryst.* **A24**, 212–216.

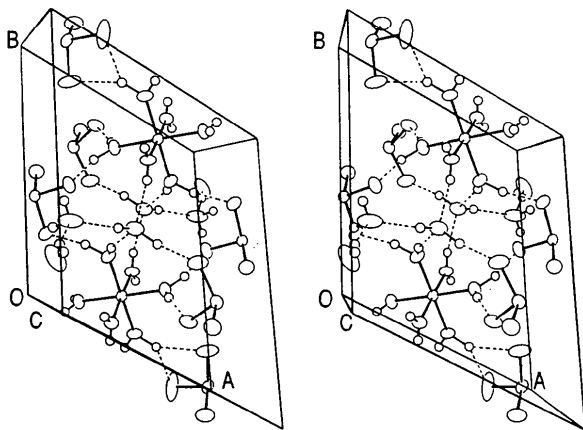


Fig. 1. Stereoview of a unit cell of  $[\text{Al}(\text{H}_2\text{O})_6](\text{BrO}_3)_3 \cdot 3\text{H}_2\text{O}$  drawn using *ORTEPII* (Johnson, 1976). Thermal ellipsoids are drawn at 50% probability for all atoms except H, for which they have been set artificially small. The strongest hydrogen bonds (those with lengths less than 2.2 Å) are shown as dashed lines.