the ac plane along the b axis is depicted in Fig. 2. The main feature of this structure is the coexistence of two different anions in the same crystal.

The $Te(OH)_6$ octahedra can be described as belonging to a number of sheets:

– sheets parallel to (001), $c/2$ apart. Each sheet includes Te atoms of one site only. The orientation of the octahedra changes from one site to another. As a consequence, each sheet is built up from octahedra which all have the same orientation; this orientation changes from one sheet to another;

– sheets parallel to (001), $(b + c)/2$ apart. These sheets include Te atoms occupying the two sites;

– sheets parallel to $(1\bar{1}0)$, $(a - b)/2$ apart. These sheets also include Te atoms occupying the two sites.

The SO_4 tetrahedra can be described as belonging to the same sheet directions, but alternating with the $Te(OH)_6$ ones.

The environment of the K atoms is octahedral:

– environment of K(1): three O atoms belonging to a Te(2) octahedron and three O atoms belonging to an SO_4 tetrahedron;

– environment of K(2): three O atoms of a Te(1) octahedron, one O atom of another Te(1) octahedron, one O atom of an SO_4 tetrahedron and one O atom of a Te(2) octahedron.

The planes (101) (Fig. 2) and $(01\bar{1})$ (not represented) contain $Te(OH)_6$ octahedra alternating with SO_4 tetrahedra. This occurrence has already been encountered in describing the sodium sulfate–tellurate compound $Te(OH)_6.Na_2SO_4$ (Zilber et al., 1980). A similar arrangement can also be observed in two recently

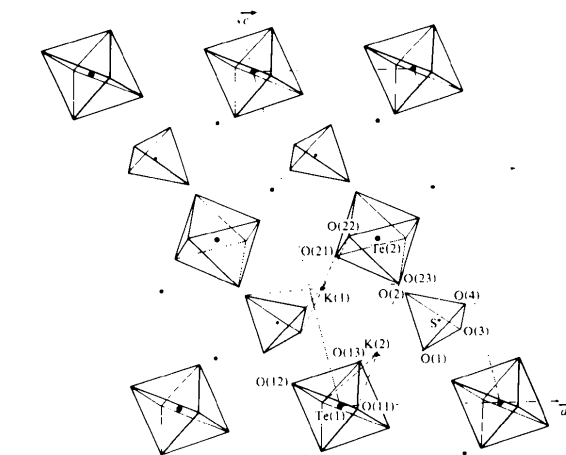Fig. 2. Projection of $Te(OH)_6.K_2SO_4$ on the ac plane along the b axis.

described phosphate–tellurate compounds: $Te(OH)_6.$ $Na_2HPO_4.H_2O$ (Durif et al., 1979) and $Te(OH)_6.$ $Na_2HPO_4.NaH_2PO_4$ (Averbuch-Pouchot, 1980), although in the last one no pure sheets of $Te(OH)_6$ octahedra are found.

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Octaaquastrontium(II) Decabromodibismuthate(III)

By F. LAZARINI AND I. LEBAN

Department of Chemistry, Faculty of Natural Sciences and Technology, University Edvard Kardelj of Ljubljana, Murnikova 6, 61000 Ljubljana, Yugoslavia

Abstract. $[Sr(H_2O)_8]_2[Bi_2Br_{10}]$, orthorhombic, Pbam, $a = 15.727$ (5), $b = 12.328$ (6), $c = 9.521$ (3) Å, $D_o = 3.03$ (2), $Z = 2$, $D_c = 3.022$ Mg m^{-3}; $R = 0.093$ for 582 diffractometer data $[I > 2.5\sigma(I)]$. The structure consists of isolated $[Sr(H_2O)_8]^{2+}$ cations, in which the H_2O molecules are arranged in the form of a square antiprism, and binuclear $[Bi_2Br_{10}]^{4-}$ anions with two $BiBr_6$ octahedra sharing an edge.

Introduction. This work is part of a systematic investigation of the stereochemical behaviour of hexahalobismuthate(III) groups in the presence of various cations (Lazarini, 1977a,b,c,d, 1978). A great variety of different halobismuthate(III) anions, most of them bi-

or polynuclear, have been observed. The linking of the hexahalobismuthate(III) groups into polynuclear species is presumably influenced by the size of the cation; therefore, further bromobismuthate(III) compounds with different cations were synthesized and characterized in order to study their crystal structures.

Yellow crystals of the title compound were grown by slow evaporation from an aqueous solution obtained by dissolving $Bi(OH)_3$ and $SrCO_3$ in a dilute HBr solution. The Bi:Sr ratio was varied from 1:2 to 2:1. The title compound was the only solid compound obtained. Its empirical formula was determined by standard chemical analytical methods (calculated: 24.87% Bi, 47.55% Br, 17.15% H_2O; found: 24.2% Bi, 48.1%

Br, 18·0% H_2O). A well developed crystal, selected for the diffraction measurements, was characterized by the following planes (in parentheses are the distances from the crystal faces to an arbitrary origin inside the crystal): $\pm(\bar{1}10)$ (0·065 mm), $\pm(110)$ (0·125 mm) and $\pm(001)$ (0·380 mm).

The intensity data were collected at 293 (1) K with an Enraf–Nonius CAD-4 diffractometer. Experimental conditions were: graphite-monochromatized Mo $K\alpha$ radiation ($\lambda = 0·71079$ Å), ω–2θ scan, $\theta_{min} = 1°$, $\theta_{max} = 25°$, 2θ scan width = $(1·0 + 0·6 \tan \theta)°$, aperature = $(2·5 + 0·9 \tan \theta)$ mm, maximum scan time 40 s, background = $\frac{1}{4}$ of the scan time at each of the scan limits. 1117 independent reflexions were recorded and of these 582 with $I > 2·5\sigma(I)$ (calculations based on counting statistics) were used in the refinement. Corrections were applied for Lorentz and polarization effects and for absorption [μ(Mo $K\alpha$) = 23·69 mm^{-1}]. The transmission factors, calculated with the measured crystal dimensions (2752 grid points, crystal volume 0·0255 mm^3), range from 0·011 to 0·079. The unit-cell parameters were obtained from a least-squares fit of the θ values of 25 reflexions measured on the diffractometer. The systematic absences (0kl: $k = 2n + 1$; $h0l$: $h = 2n + 1$), checked by Weissenberg and precession photographs, and the clearly centrosymmetric distribution of the normalized structure factors indicated the space group $Pbam$, which was subsequently confirmed by the successful refinement.

The positions of the Bi, Br and Sr atoms were determined from the three-dimensional Patterson map, while the O atoms of the water molecules were located from a difference Fourier summation. The structure was refined by the full-matrix least-squares technique with anisotropic thermal parameters for Bi, Br and Sr atoms, isotropic for O atoms and with an anomalous-dispersion correction for all atoms. The function minimized in the least-squares procedure was $\sum w(|F_o|$

$- |F_c|)^2$. The weighting function applied in the final cycle was $w = 1·39[\sigma(F_o)^2 - 0·0104F_o^2]$. An empirical extinction parameter was also included in the final stage of the refinement; its value in the final cycle was 3·1 (1) $\times 10^{-3}$. Final R values are $R = \sum ||F_o| - |F_c||/\sum |F_o| = 0·093$ and $R_w = [\sum w(F_o - F_c)^2/\sum wF_o^2]^{1/2} = 0·129$ for 582 reflexions and 60 parameters. The average parameter shift-to-error ratio was 0·044 in the final cycle. A final difference Fourier map was featureless.

All calculations were performed on the CDC Cyber 172 computer of RRC Ljubljana with *SHELX* 76 (Sheldrick, 1976). Atomic scattering factors for neutral atoms tabulated by Cromer & Mann (1968) and the values of f' and f'' for the anomalous-dispersion correction of Cromer & Liberman (1970) were applied.

The positional and thermal parameters are listed in Table 1.* Equivalent isotropic thermal parameters are

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35456 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
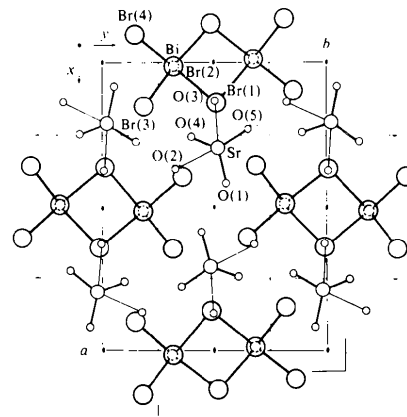

Fig. 1. Projection of the structure of $|Sr(H_2O)_8|_2|Bi_2Br_{10}|$ along c.

Table 1. *Final positional parameters* ($\times 10^4$, *for* O $\times 10^3$) *and thermal parameters* (Å^2 $\times 10^3$) *with standard deviations in parentheses*

For Bi, Br and Sr atoms the equivalent isotropic thermal parameter is given [calculated as $U_{eq} = (U_{11} \cdot U_{22} \cdot U_{33})^{1/3}$], for O atoms the isotropic thermal parameter is given.

	x	y	z	U_{eq} or U
Bi	105 (2)	3186 (3)	0	36 (2)
Br(1)	1311 (6)	5126 (8)	0	55 (6)
Br(2)	92 (6)	3223 (8)	2979 (6)	72 (5)
Br(3)	1501 (7)	1884 (11)	0	78 (7)
Br(4)	−1001 (8)	1482 (10)	0	88 (9)
Sr	2932 (6)	5172 (8)	5000	51 (5)
O(1)	416 (3)	553 (5)	333 (6)	98 (17)
O(2)	369 (5)	328 (7)	500	108 (27)
O(3)	126 (6)	506 (8)	500	140 (35)
O(4)	254 (3)	397 (5)	276 (7)	106 (18)
O(5)	227 (4)	651 (6)	306 (7)	121 (22)

Table 2. *Interatomic distances* (Å) *and angles* (°) *with standard deviations in parentheses*

Sr—O(1),O(1^i)	2·54 (5)	Br(2)—Bi—Br(1)	89·5 (2)
Sr—O(2)	2·62 (8)	Br(2^{iii})—Bi—Br(1)	89·5 (2)
Sr—O(3)	2·64 (10)	Br(2)—Bi—Br(1^{ii})	89·1 (2)
Sr—O(4),O(4^i)	2·67 (6)	Br(2^{iii})—Bi—Br(1^{ii})	89·1 (2)
Sr—O(5),O(5^i)	2·69 (7)	Br(2)—Bi—Br(3)	90·9 (2)
		Br(2^{iii})—Bi—Br(3)	90·9 (2)
Bi—Br(1)	3·05 (1)	Br(2)—Bi—Br(4)	90·4 (2)
Bi—Br(1^{ii})	3·05 (1)	Br(2^{iii})—Bi—Br(4)	90·4 (2)
Bi—Br(2),Br(2^{iii})	2·837 (6)	Br(2)—Bi—Br(2^{iii})	178·0 (3)
Bi—Br(3)	2·72 (1)	Br(1)—Bi—Br(3)	87·8 (3)
Bi—Br(4)	2·73 (1)	Br(1)—Bi—Br(4)	178·8 (3)
		Br(1^{ii})—Bi—Br(3)	173·1 (4)
Br(2)—Br(2^i)	3·848 (8)	Br(1^{ii})—Bi—Br(4)	93·4 (3)
O(1)—O(1^{iv})	2·95 (7)	Br(3)—Bi—Br(4)	93·5 (4)
		Bi—Br(1)—Bi^{ii}	94·6 (3)

Symmetry code

(i)	$x, y, 1 - z$	(ii)	$-x, 1 - y, -z$
(iii)	$x, y, -z$	(iv)	$1 - x, 1 - y, z$

given for Bi, Br and Sr atoms and isotropic thermal parameters for O atoms. A projection of the structure along c and the atom-numbering system used are shown in Fig. 1. Some important interatomic distances and angles are given in Table 2.

Discussion. The structure of $|Sr(H_2O)_8|_2|Bi_2Br_{10}|$ consists of isolated octaaquastrontium(II) cations and binuclear decabromodibismuthate(III) anions. The anions and cations, arranged parallel to the xy plane, alternate at $z = 0$ and $\frac{1}{2}$.

The anion is composed of two $BiBr_6$ octahedra sharing an edge. The two Bi atoms, the two bridging Br atoms and four of the terminal Br atoms are on a mirror plane. The distances from the Bi atom to the terminal Br atoms in *trans* positions with respect to the bridging Br atoms are slightly shorter [2·72 (1) Å] than the distances to the remaining terminal Br atoms, which are not on the mirror plane [2·837 (6) Å]. The distances from the Bi atom to the bridging Br atoms are longer [3·05 (1) Å]. Close contacts shorter than the sum of the van der Waals radii (3·90 Å; Wells, 1975) are present between Br atoms of different layers [Br(2)–Br(2^i), 3·848 (8) Å]. The bond distances and angles within the $|Bi_2Br_{10}|^{4-}$ anion are very similar to those found in the crystal structure of $K_4|Bi_2Br_{10}|.4H_2O$ and in the isomorphous ammonium compound. However, the anions in these compounds have a different crystallographic symmetry: only the bridging Br atoms are on a mirror plane; the Bi—Br(terminal) distances are 2·749 (3), 2·784 (3) Å and 2·809 (3), 2·879 (3) Å, and the Bi—Br(bridging) distances are 2·979 (2) and 3·006 (2) Å. Although the anions are similar, the crystal structure is entirely different; in the K compound as well as the H_2O molecules some of the Br atoms are coordinated to the K atoms, while in the Sr compound only the H_2O molecules are coordinated to the Sr atoms.

The coordination polyhedron of $|Sr(H_2O)_8|^{2+}$ is a slightly distorted square antiprism, shown schematically in Fig. 2. The bond distances within the cation
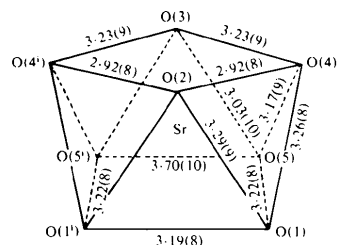

Fig. 2. A schematic representation of the $|Sr(H_2O)_8|^{2+}$ cation.

are given in Table 2 while in Fig. 2 some other illustrative interatomic distances are shown. Hydrogen bonds between H_2O molecules of different cations do not seem to be present [the shortest distance between two O atoms of different cations is O(1)–O(1^{iv}), 2·95 (7) Å].

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