

Table 3. Survey of known structures containing different types of coexisting anions

Types of coexisting anions	Associated compounds	Reference
$(\text{CrO}_4)^{2-}$ – $(\text{Cr}_2\text{O}_7)^{2-}$ $(\text{NO}_3)^-$ – $(\text{PO}_4)^{3-}$	$\left\{ \begin{array}{l} \text{Fe}(\text{CrO}_4)_2, \text{Cr}_2\text{O}_7, 4\text{H}_2\text{O} \\ \alpha\text{-Al}_2(\text{CrO}_4)_3, \text{Cr}_2\text{O}_7, 4\text{H}_2\text{O} \\ \text{HgNO}_3, \text{PO}_4, \text{H}_2\text{O} \end{array} \right\}$	Gérault & Bonnin (1976) Cudennec (1977) Durif, Tordjman, Masse & Guitel (1978)
$(\text{P}_2\text{O}_7)^{4-}$ – $(\text{P}_3\text{O}_{10})^{5-}$	$(\text{NH}_4)_2\text{Cd}_6(\text{P}_2\text{O}_7)_2(\text{P}_3\text{O}_{10})$	Ivanov, Simonov & Belov (1978)
$(\text{PO}_4)^{3-}$ – $(\text{TeO}_6)^{6-}$	$\left\{ \begin{array}{l} \text{Te}(\text{OH})_6, 2(\text{NH}_4)_2\text{HPO}_4 \\ \text{Te}(\text{OH})_6, \text{Na}_2\text{HPO}_4, \text{H}_2\text{O} \\ \text{Te}(\text{OH})_6, \text{Rb}_2\text{HPO}_4, \text{RbH}_2\text{PO}_4 \end{array} \right\}$	Durif, Averbuch-Pouchot & Guitel (1979) Averbuch-Pouchot, Durif & Guitel (1979)
$(\text{AsO}_4)^{3-}$ – $(\text{TeO}_6)^{6-}$	$\left\{ \begin{array}{l} \text{Te}(\text{OH})_6, \text{Na}_2\text{HAsO}_4, \text{H}_2\text{O} \\ \text{Te}(\text{OH})_6, \text{Rb}_2\text{HAsO}_4, \text{RbH}_2\text{AsO}_4 \\ \text{Te}(\text{OH})_6, 2(\text{NH}_4)_2\text{HAsO}_4 \end{array} \right\}$	Averbuch-Pouchot & Durif (1980)
$(\text{SO}_4)^{2-}$ – $(\text{TeO}_6)^{6-}$	$\text{Te}(\text{OH})_6, \text{Na}_2\text{SO}_4$	This work

Table 4. Positional parameters of the hydrogen atoms belonging to the hydroxyl groups

	x	y	z
H(1)	0.54	–0.01	0.485
H(2)	0.84	0.47	0.12
H(3)	0.32	0.26	0.51
H(4)	0.35	0.036	0.62
H(5)	0.20	0.12	0.87
H(6)	0.44	0.29	0.93

A small number of cases of different types of anions coexisting in the same crystal have already been reported. A brief survey of such compounds is given in Table 3 indicating the types of anions taking part. The shortest Te–Te distance in the present salt is 5.459 (5) Å (the smallest cell dimension). This is the shortest

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## Structure of Potassium Sulfate Tellurate: $\text{Te}(\text{OH})_6 \cdot \text{K}_2\text{SO}_4$

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**Abstract.**  $\text{Te}(\text{OH})_6 \cdot \text{K}_2\text{SO}_4$ , triclinic,  $P\bar{1}$ ,  $a = 6.243$  (2),  $b = 6.647$  (2),  $c = 13.405$  (2) Å,  $\alpha = 73.14$  (5),  $\beta = 103.05$  (5),  $\gamma = 116.97$  (5)°,  $V = 472$  (2) Å<sup>3</sup>,  $Z = 2$ ,  $D_x = 3.07$  Mg m<sup>–3</sup>. The structure has been determined using the Patterson method and refined to an  $R$  value of 0.048 with 3037 independent reflections. The main interest of this structure is the presence of two different types of anions in the same crystal.

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among the compounds surveyed in Table 3: such distances are usually substantially longer.

Calculations of the bond strengths based on the work of Brown & Shannon (1973) and Donnay & Allman (1970), and assuming a linear O–H···O bond, led to the positions of the H atoms of the hydroxyl groups, as indicated in Table 4. For clarity, the position of H(1) is depicted only on the  $ab$  projection (Fig. 1), those of H(3), H(4), H(5) and H(6) only on the  $bc$  projection (Fig. 2), and that of H(2) is shown on both projections. The positions are all compatible with the usual positions of such H atoms.

The next compound of the series to be investigated in this laboratory is the potassium salt:  $\text{Te}(\text{OH})_6 \cdot \text{K}_2\text{SO}_4$ .

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**Introduction.** The crystal structure determination presented in this paper is part of a systematic investigation on alkali phosphate and sulfate–tellurate salts (Durif, Averbuch-Pouchot & Guitel, 1979; Averbuch-Pouchot, Durif & Guitel, 1979; Zilber, Tordjman & Guitel, 1980). The chemical preparation and characteristic powder data of the title compound are to be published elsewhere.

A preliminary analysis by the Weissenberg method showed that the crystal was triclinic. The space group

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$P\bar{1}$  was assumed with  $Z = 2$  and this was confirmed by the final result.

The crystal used for the structure determination was a small, almost cubic, prism  $0.12 \times 0.12 \times 0.12$  mm. 3916 reflections were recorded on a Philips PW 1100 four-circle diffractometer. The radiation used was that from a silver target [ $\lambda(\text{Ag } K\alpha) = 0.5608 \text{ \AA}$ ], monochromatized with a graphite plate. Measurements were run between  $3$  and  $30^\circ$  ( $\theta$ ) with a scan speed of  $0.03^\circ \text{ s}^{-1}$  and a scan width of  $1.30^\circ$ . The background was measured for 10 s at each edge of the scan range; the  $\omega$ -scan mode was used. Because of the small size of the crystal, and the radiation used, no absorption correction was made; a Lorentz-polarization correction was applied to the data.

The structure was solved using the heavy-atom method. A Patterson function allowed two Te atoms to be placed in special positions. A Fourier synthesis gave an  $R$  factor of 0.28 and allowed positioning of the S atoms, one K atom and most of the O atoms. A few more least-squares refinements and a difference Fourier synthesis gave the positions of the second K atom and the remaining O atoms.

Finally, the unweighted  $R$  factor ( $R = \sum |F_o| - |F_c| / \sum |F_o|$ ) reduced to a value of 0.048 and the weighted  $R$  factor ( $R_w = [\sum w(|F_o| - |F_c|)^2 / \sum wF_o^2]^{1/2}$ ) to 0.103 with 3037 independent reflections [ $I > 3\sigma(I)$ ]. The quantity minimized was  $\sum w(|F_o| - |F_c|)^2$  with  $w = \sigma^{-2}(F_o)$  determined by counting statistics.

Table 1 gives the positional and  $B_{\text{eq}}$  parameters with their estimated standard deviations and Table 2 the main interatomic distances and bond angles.\*

**Discussion.** Fig. 1 shows a projection on the  $ab$  plane along the  $c$  axis of  $\text{Te}(\text{OH})_6 \cdot \text{K}_2\text{SO}_4$ . A projection on

\* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35535 (24 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Positional parameters ( $\times 10^4$ ) with their estimated standard deviations and equivalent isotropic thermal parameters

	$x$	$y$	$z$	$B_{\text{eq}}$ ( $\text{\AA}^2$ )
Te(1)	0	0	0	0.78
Te(2)	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.84
S	7488 (4)	2845 (3)	2516 (2)	0.86
K(1)	784 (5)	8826 (5)	3505 (3)	1.83
K(2)	3061 (5)	5915 (5)	1497 (3)	1.96
O(11)	1063 (14)	3262 (12)	9893 (7)	1.22
O(12)	7304 (14)	9371 (13)	690 (7)	1.52
O(13)	1936 (15)	9782 (14)	1330 (7)	1.40
O(21)	2086 (16)	2707 (15)	4436 (8)	1.84
O(22)	3228 (15)	6656 (15)	5075 (8)	1.76
O(23)	5613 (16)	6787 (15)	3587 (7)	1.69
O(1)	6034 (14)	3692 (15)	1593 (8)	1.76
O(2)	5835 (16)	1201 (16)	3314 (7)	1.76
O(3)	8650 (16)	1638 (15)	2179 (8)	2.05
O(4)	9394 (18)	4771 (16)	2938 (9)	2.30

Table 2. Interatomic distances and angles

The  $\text{Te}(i)\text{—O}(j)$  and  $\text{S—O}(i)$  distances are in  $\text{\AA}$ , and are underlined in the diagonals. Below the diagonals the  $\text{O}(i)\text{—S—O}(j)$  and  $\text{O}(ij)\text{—Te}(i)\text{—O}(ik)$  angles are given in degrees and  $\frac{1}{10}^\circ$ . Above the diagonals, the  $\text{O—O}$  distances are given in  $\text{\AA}$ . The estimated standard deviations are given in parentheses.

(a) The Te(1) octahedron

Te(1)	O(11)	O(12)	O(13)
O(11)	<u>1.928 (4)</u>	2.713 (5)	2.728 (6)
O(12)	89.5 (2)	<u>1.925 (4)</u>	2.707 (7)
O(13)	90.2 (2)	90.6 (2)	<u>1.922 (4)</u>

(b) The Te(2) octahedron

Te(2)	O(21)	O(22)	O(23)
O(21)	<u>1.933 (4)</u>	2.709 (7)	2.749 (7)
O(22)	90.5 (2)	<u>1.914 (5)</u>	2.706 (9)
O(23)	89.5 (2)	89.3 (2)	<u>1.938 (5)</u>

(c) The  $\text{SO}_4$  tetrahedron

S	O(1)	O(2)	O(3)	O(4)
O(1)	<u>1.492 (5)</u>	2.410 (6)	2.443 (8)	2.417 (6)
O(2)	108.2 (3)	<u>1.483 (5)</u>	2.444 (9)	2.419 (6)
O(3)	109.4 (3)	109.9 (3)	<u>1.503 (5)</u>	2.393 (8)
O(4)	110.4 (3)	111.00 (4)	108.1 (4)	<u>1.453 (5)</u>

(d) The environment of the K atoms

K(1)—O(21 <sup>I</sup> )	2.895 (5)	K(2)—O(11 <sup>I</sup> )	2.878 (5)
K(1)—O(22 <sup>I</sup> )	2.761 (5)	K(2)—O(12 <sup>I</sup> )	2.792 (5)
K(1)—O(23 <sup>I</sup> )	2.894 (5)	K(2)—O(13 <sup>I</sup> )	2.896 (5)
K(1)—O(2 <sup>I</sup> )	2.849 (5)	K(2)—O(11 <sup>II</sup> )	2.987 (5)
K(1)—O(3 <sup>I</sup> )	2.773 (6)	K(2)—O(23 <sup>I</sup> )	2.969 (6)
K(1)—O(4 <sup>I</sup> )	2.713 (6)	K(2)—O(1 <sup>I</sup> )	2.813 (5)

The code for the atoms: The arabic numerals, (1) through (4), (11) through (13) and (21) through (23), correspond to crystallographically independent atoms. The roman numerals correspond to the following positions: (I)  $x, y, z$ ; (II)  $\bar{x}, \bar{y}, \bar{z}$ .

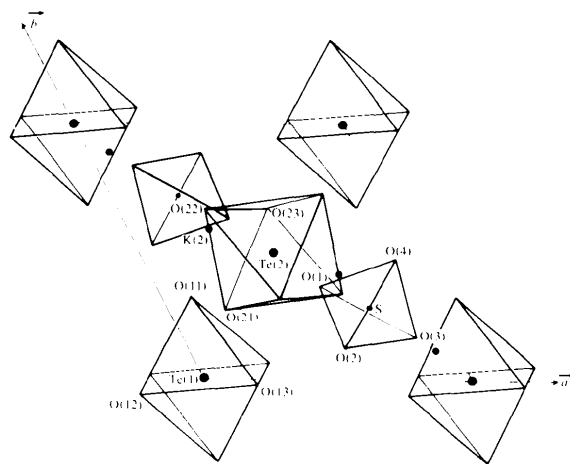


Fig. 1. Projection of  $\text{Te}(\text{OH})_6 \cdot \text{K}_2\text{SO}_4$  on the  $ab$  plane along the  $c$  axis.

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  $\text{Te}(\text{OH})_6$  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 (110),  $(a - b)/2$  apart. These sheets also include Te atoms occupying the two sites.

The  $\text{SO}_4$  tetrahedra can be described as belonging to the same sheet directions, but alternating with the  $\text{Te}(\text{OH})_6$  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  $\text{SO}_4$  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  $\text{SO}_4$  tetrahedron and one O atom of a Te(2) octahedron.

The planes (101) (Fig. 2) and (011) (not represented) contain  $\text{Te}(\text{OH})_6$  octahedra alternating with  $\text{SO}_4$  tetrahedra. This occurrence has already been encountered in describing the sodium sulfate–tellurate compound  $\text{Te}(\text{OH})_6 \cdot \text{Na}_2\text{SO}_4$  (Zilber *et al.*, 1980). A similar arrangement can also be observed in two recently

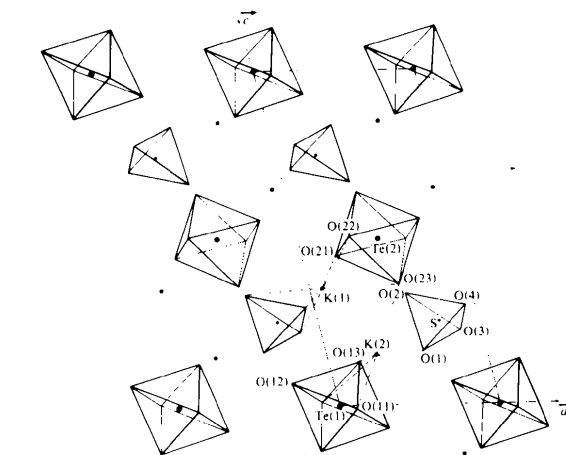


Fig. 2. Projection of  $\text{Te}(\text{OH})_6 \cdot \text{K}_2\text{SO}_4$  on the  $ac$  plane along the  $b$  axis.

described phosphate–tellurate compounds:  $\text{Te}(\text{OH})_6 \cdot \text{Na}_2\text{HPO}_4 \cdot \text{H}_2\text{O}$  (Durif *et al.*, 1979) and  $\text{Te}(\text{OH})_6 \cdot \text{Na}_2\text{HPO}_4 \cdot \text{NaH}_2\text{PO}_4$  (Averbuch-Pouchot, 1980), although in the last one no pure sheets of  $\text{Te}(\text{OH})_6$  octahedra are found.

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## Octaaquastrontium(II) Decabromodibismuthate(III)

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**Abstract.**  $[\text{Sr}(\text{H}_2\text{O})_8]_2[\text{Bi}_2\text{Br}_{10}]$ , 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<sup>-3</sup>;  $R = 0.093$  for 582 diffractometer data [ $I > 2.5\sigma(I)$ ]. The structure consists of isolated  $[\text{Sr}(\text{H}_2\text{O})_8]^{2+}$  cations, in which the  $\text{H}_2\text{O}$  molecules are arranged in the form of a square antiprism, and binuclear  $[\text{Bi}_2\text{Br}_{10}]^{4-}$  anions with two  $\text{BiBr}_6$  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, 1977*a,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  $\text{Bi}(\text{OH})_3$  and  $\text{SrCO}_3$  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%  $\text{H}_2\text{O}$ ; found: 24.2% Bi, 48.1%