

atom positions, but there are no significant differences with respect to the Mn and S coordination.

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## Structure of Sodium Sulfate Tellurate

BY R. ZILBER,\* I. TORDJMAN AND J. C. GUITEL

*Laboratoire de Cristallographie, CNRS, 166 X, 38042 Grenoble CEDEX, France*

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**Abstract.**  $\text{Te}(\text{OH})_6 \cdot \text{Na}_2\text{SO}_4$ , monoclinic, *Cc*,  $a = 5.459$  (5),  $b = 10.306$  (7),  $c = 15.349$  (10) Å,  $\beta = 94.73$  (5)°,  $V = 861$  (2) Å<sup>3</sup>,  $Z = 4$ ,  $D_x = 2.87$  Mg m<sup>-3</sup>. The structure has been determined using the Patterson method and refined to an *R* value of 0.027 for 2431 independent reflections. The interest of this structure is the presence of two different anions in the same crystal.

**Introduction.** This study is part of a systematic investigation of alkali phosphate- and sulfate-tellurate salts. The chemical preparation and crystal data of the title compound have been reported elsewhere (Zilber, 1980).

A piezo-electric test on the crystal proved to be inconclusive so that doubt remained as to whether the correct space group is *C2/c* or *Cc*.

The crystal used was a small, almost cubic prism of approximate dimensions 0.12 × 0.12 × 0.12 mm. 2476 reflections were recorded on a Philips PW 1100 four-circle diffractometer equipped with a graphite monochromator. The radiation used was that of a silver anticathode [ $\lambda(\text{Ag } K\alpha) = 0.5608$  Å]. The angular range was taken between 3 and 23° ( $\theta$ ), the scan speed was 0.02° s<sup>-1</sup> and the scan width 1.30°. The background was measured for 10 s at each end of the scan range. An  $\omega$  scan was used. Because of the small size of the crystal and the radiation used, no correction for absorption was made. Nevertheless, a Lorentz-polarization correction was applied to the data.

\*On leave from Soreq Nuclear Research Centre, Yavne, Israel.

The structure was solved using the heavy-atom method. A Patterson function allowed the location of the Te atoms. A Fourier synthesis gave an *R* factor of 0.53 and allowed the positioning of the O atoms, thus confirming the space group *Cc*. A few more refinements gave the positions of the S and Na atoms. Finally, the unweighted *R* ( $R = \sum |F_o| - |F_c| / \sum |F_o|$ ) came down to a value of 0.027 and the weighted *R* ( $R_w = [\sum w(|F_o| - |F_c|)^2 / \sum wF_o^2]^{1/2}$ ) to a value of 0.039 for 2431 independent reflections. The quantity minimized was  $\sum w(|F_o| - |F_c|)^2$  with  $w = \sigma^{-2}(F_o)$  determined by counting statistics. The reflections had  $I > 3\sigma(I)$ .

Table 1. *Positional parameters* ( $\times 10^4$ ) *with their estimated standard deviations, and*  $B_{\text{eq}}$  *for*  $\text{Te}(\text{OH})_6 \cdot \text{Na}_2\text{SO}_4$

	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{eq}}$ (Å <sup>2</sup> )
Te	0	77 (2)	0	0.63
S	3873 (3)	2457 (1)	7483.7 (9)	0.85
Na(1)	3405 (5)	2455 (3)	1216 (2)	1.42
Na(2)	4589 (6)	747 (3)	3104 (2)	1.64
O(1)	2092 (9)	3250 (5)	6937 (3)	1.45
O(2)	6353 (8)	3005 (6)	7460 (3)	1.72
O(3)	3799 (10)	1116 (5)	7175 (3)	1.69
O(4)	3063 (9)	2509 (5)	8392 (3)	1.42
O(1H)	1764 (9)	4877 (7)	4422 (3)	2.35
O(2H)	8235 (6)	4861 (4)	5613 (2)	0.69
O(3H)	4942 (9)	3072 (4)	5194 (3)	1.35
O(4H)	3631 (8)	5318 (4)	6088 (3)	1.19
O(5H)	6386 (8)	4736 (4)	3927 (3)	1.24
O(6H)	5383 (8)	6770 (4)	4890 (2)	1.08

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

The  $\text{SO}(i)$  and  $\text{TeO}(i\text{H})$  distances are given (underlined) along the diagonals. Below the diagonals, the angles  $\text{O}(i)\text{SO}(i)$  and  $\text{O}(i\text{H})\text{TeO}(j\text{H})$  are given. Above the diagonals, the O—O distances are given. The estimated standard deviations are given in parentheses. The Arabic numerals, 1 through 6, correspond to crystallographically independent atoms. The Roman numerals correspond to the following positions: (I)  $x, y, z$ ; (II)  $x, y, \frac{1}{2} + z$ ; (III)  $\frac{1}{2} + x, \frac{1}{2} + y, z$ ; (IV)  $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$ .

(a)  $\text{SO}_4$  tetrahedron

S	O(1)	O(2)	O(3)	O(4)
O(1)	<u>1.477 (5)</u>	2.411 (6)	2.404 (7)	2.377 (7)
O(2)	109.8 (3)	<u>1.470 (5)</u>	2.414 (7)	2.440 (7)
O(3)	109.9 (3)	110.9 (3)	<u>1.461 (5)</u>	2.416 (7)
O(4)	106.1 (3)	110.6 (3)	109.5 (3)	<u>1.497 (5)</u>

(b)  $\text{Te}(\text{OH})_6$  octahedron

Te	O(1H)	O(2H)	O(3H)	O(4H)	O(5H)	O(6H)
O(1H)	<u>1.911 (5)</u>	2.764 (7)	2.745 (8)	2.713 (7)	2.698 (7)	2.827 (8)
O(2H)	176.4 (2)	<u>1.932 (3)</u>	2.618 (6)	2.715 (6)	2.702 (5)	2.690 (5)
O(3H)	91.2 (2)	85.3 (1)	<u>1.931 (4)</u>	2.813 (6)	2.757 (6)	3.849 (6)
O(4H)	89.9 (2)	89.4 (1)	93.6 (2)	<u>1.928 (4)</u>	3.801 (6)	2.612 (6)
O(5H)	90.8 (2)	90.3 (1)	92.7 (2)	173.6 (2)	<u>1.879 (4)</u>	2.648 (6)
O(6H)	95.0 (2)	88.5 (1)	173.8 (2)	85.4 (2)	88.3 (2)	<u>1.924 (4)</u>

(c) Environment of the  $\text{Na}^+$  ions

Na(1)—O(1 <sup>IV</sup> )	2.331 (5)	Na(1)—O(3H <sup>IV</sup> )	2.417 (5)	Na(2)—O(1 <sup>IV</sup> )	2.558 (6)	Na(2)—O(4 <sup>IV</sup> )	2.624 (6)
Na(1)—O(2 <sup>IV</sup> )	2.341 (6)	Na(1)—O(4H <sup>II</sup> )	2.308 (5)	Na(2)—O(2 <sup>IV</sup> )	2.337 (6)	Na(2)—O(1H <sup>III</sup> )	2.431 (6)
Na(1)—O(2H <sup>IV</sup> )	2.559 (5)	Na(1)—O(6H <sup>II</sup> )	2.511 (5)	Na(2)—O(3 <sup>II</sup> )	2.409 (6)	Na(2)—O(5H <sup>III</sup> )	2.470 (6)

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

**Discussion.** Fig. 1 shows a projection on the  $ab$  plane of  $\text{Te}(\text{OH})_6 \cdot \text{Na}_2\text{SO}_4$ . A projection on the  $bc$  plane is depicted in Fig. 2. The main feature of this structure is

\* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35358 (20 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

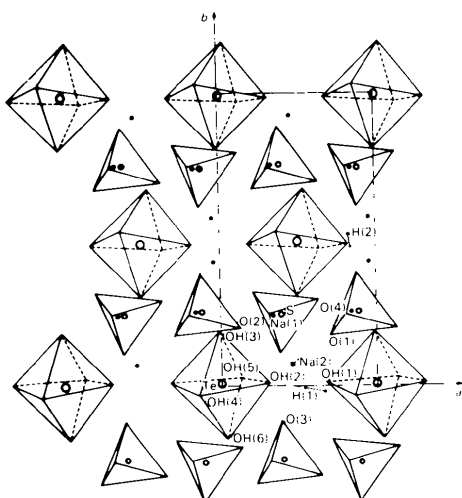


Fig. 1. Projection of  $\text{Te}(\text{OH})_6 \cdot \text{Na}_2\text{SO}_4$  on the  $ab$  plane. For clarity, only one of the two Te octahedra projected in the same area is depicted:  $\text{Te}(0,0,\frac{1}{2})$ ,  $\text{Te}(0,\frac{1}{2},0)$  and  $\text{Te}(0,1,0)$  are omitted.

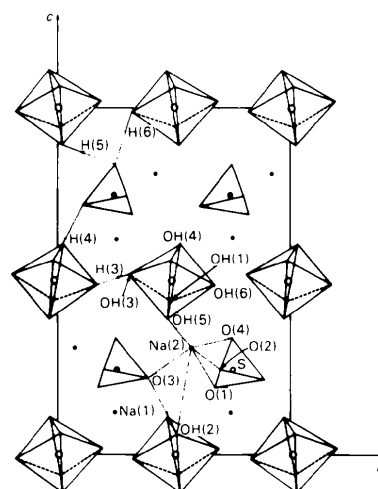


Fig. 2. Projection of  $\text{Te}(\text{OH})_6 \cdot \text{Na}_2\text{SO}_4$  on the  $bc$  plane.

the presence of two different anions in the same crystal. The  $\text{Te}(\text{OH})_6$  octahedra belong to sheets perpendicular to the  $c$  axis, alternating with sheets of  $\text{SO}_4$  tetrahedra also perpendicular to the  $c$  axis. Similarly, parallel sheets of either pure  $\text{Te}(\text{OH})_6$  octahedra or pure  $\text{SO}_4$  tetrahedra intercalate perpendicular to the  $b$  axis. The  $\text{Na}^+$  cations have an octahedral coordination and are distributed between two sites. In one of them, the Na is coordinated by two O atoms belonging to S tetrahedra and four OH groups belonging to Te octahedra, whereas the situation is reversed for the Na at the other site: four O atoms belonging to S tetrahedra and two OH groups belonging to Te octahedra constitute its coordination polyhedron.

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: $\text{Te}(\text{OH})_6 \cdot \text{K}_2\text{SO}_4$

BY R. ZILBER,\* A. DURIF AND M. T. AVERBUCH-POUCHOT

*Laboratoire de Cristallographie, CNRS, 166 X, 38042 Grenoble CEDEX, France*

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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.

\* On leave from: Soreq Nuclear Research Centre, Yavne, Israel.

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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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