approximately along the bond direction (Fig. 1). The angle between this component and the O(5)···O(2) direction is 25° [the O(5)—D(2)···O(2) angle is 176°]. For the other two D atoms the largest r.m.s. component (0·171 and 0·185 Å) is in each case closer to a right angle to the O···O bond direction (Fig. 1); the angles are 56 and 102°, respectively. These observations, together with the large isotope effect for D(2), indicate that D(2) is situated in a shallow skew potential well.

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Structure of Thallium Sulfate Tellurate $Te(OH)_6.Tl_2SO_4$

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Abstract. $Te(OH)_6.Tl_2SO_4$ is monoclinic, $P2_1/a$, with $a = 12.053$ (5), $b = 7.205$ (1), $c = 12.354$ (6) Å, $\beta = 110.85$ (5)°, $V = 1003$ (1) Å^3, $Z = 4$, $D_x = 4.87$ Mg m^{-3}. The structure has been determined using the Patterson method and refined to an R of 0·055 for 1399 independent reflections. The main interest of this structure lies in the presence of two different types of anions in the crystal. A difficulty arose in the structure determination due to the occurrence of two heavy atoms in the crystal.

Introduction. Like the other sulfate tellurate salts of this series (Zilber, Tordjman & Guitel, 1980; Zilber, Durif & Averbuch-Pouchot, 1980, 1981) the title compound was obtained as crystals grown from solution.

A piezoelectric test was inconclusive and a preliminary photographic study by the Weissenberg method showed monoclinic symmetry. Not much effort was invested in the analysis of the photographs since the data collection confirmed the unit cell measured on the film and showed unambiguously the systematic extinctions of the monoclinic space group $P2_1/a$, which are: hkl: no conditions; $h0l$: $h = 2n + 1$; $0k0$: $k = 2n + 1$; $h00$: $h = 2n + 1$. General positions for space group $P2_1/a$: 4(e) (i) x,y,z; (ii) $\frac{1}{2} - x, \frac{1}{2} + y, -z$; (iii) $-x,-y,-z$; (iv) $\frac{1}{2} + x, \frac{1}{2} - y, z$.

The crystal used for the data collection was a small prism of approximate dimensions 0·12 × 0·7 × 0·7 mm. 2316 reflections were recorded on a Philips PW1100 four-circle diffractometer equipped with a graphite monochromator. The radiation used was that of a silver target [λ(Ag $K\alpha$) = 0·5608 Å].

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The angular range was taken between 3 and 24°(θ), the scan speed was 0·02° s^{-1} and the scan width 1·20°. The background was measured for 10 s at each end of the scan range. An ω scan was used. The shape of the crystal did not allow a correction for absorption, the influence of which was observed on the intensities of some reflections. These were rejected in the final refinement cycles with the consequence of improving the residual factor and making positive some thermal parameters. A Lorentz–polarization correction was applied to the data.

The structure was solved using the heavy-atom method. The compound under study contained two heavy atoms and the Patterson functions showed very strong peaks at $\frac{1}{2},\frac{1}{2},0$ and $\frac{1}{2},0,\frac{1}{2}$. The Te were located first, then the Tl atoms and four O atoms. Two of the O atoms proved later to belong to the sulfur tetrahedron, the two others to one of the Te octahedra. It was only after a Fourier and a difference-Fourier map were computed that the S atom could be located. The remaining O atoms then followed, without difficulty, from more difference-Fourier maps.

Finally, the unweighted R factor ($R = \sum||F_o| - |F_c||/\sum|F_o|$) reduced to a value of 0·055 and the weighted R factor $\{R_w = [\sum w(|F_o| - |F_c|)^2/\sum wF_o^2]^{1/2}\}$ to 0·062 for 1399 independent observations such that $F > 3\sigma(F)$. The quantity minimized was $\sum w(|F_o| - |F_c|)^2$ with $w = 1/\sigma^2(F_o)$ determined by counting statistics. The computations were carried out on a PDP-11, using an SDP set of programs.

Discussion. Fig. 1 shows a projection along the c axis of $Te(OH)_6.Tl_2SO_4$. A projection along the a axis is depicted in Fig. 2. Table 1 gives the positional and B_{eq} parameters with their estimated standard deviations and Table 2 the main interatomic distances and bond angles.*

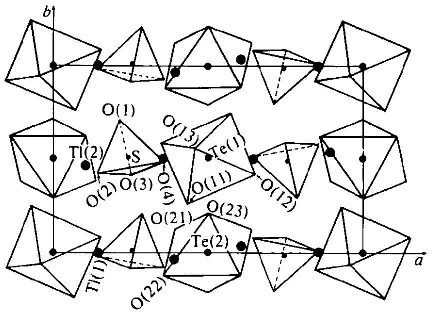

Fig. 1. Projection of $Te(OH)_6.Tl_2SO_4$ along the c axis.

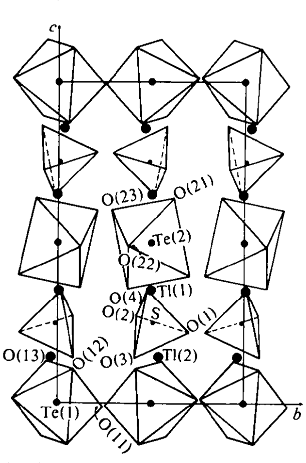

Fig. 2. Projection of $Te(OH)_6.Tl_2SO_4$ along the a axis.

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

$$B_{eq} = \frac{4}{3}\sum_i \sum_j \beta_{ij}\,\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq} (Å)
Te(1)	0	0	0	1·07 (3)
Te(2)	5000	0	5000	1·05 (3)
Tl(1)	1449 (1)	18 (2)	3514 (1)	2·61 (2)
Tl(2)	1066 (1)	4635 (2)	8569 (1)	2·53 (2)
S	2433 (4)	5106 (8)	2485 (5)	1·31 (8)
O(1)	2240 (20)	7050 (20)	2210 (20)	2·8 (4)
O(2)	3510 (20)	9250 (20)	7250 (20)	2·4 (4)
O(3)	2430 (20)	9130 (30)	8500 (20)	2·2 (3)
O(4)	3520 (20)	4870 (30)	3500 (20)	2·7 (3)
O(11)	4360 (20)	2550 (20)	9930 (20)	1·6 (3)
O(12)	1520 (20)	83 (20)	1050 (20)	2·5 (4)
O(13)	5450 (20)	4460 (30)	8680 (20)	2·6 (4)
O(21)	3960 (20)	1180 (20)	3590 (20)	1·9 (3)
O(22)	1360 (20)	3900 (50)	4860 (30)	7·3 (7)
O(23)	4990 (20)	2090 (40)	5970 (30)	5·3 (6)

The striking feature of this structure is, as in the previous structures of this series, the coexistence of two different types of anions in the same crystal.

Pure sheets of $Te(OH)_6$ octahedra are observed:

(i) Parallel to (001), **c**/2 apart. Each sheet in this direction contains Te atoms of one site only. However, the octahedra do not have the same orientation within one sheet. Nevertheless, the sheets have the same configuration, but they are located as if they were translated by **b**/2 with respect to each other.

(ii) Parallel to (100) and **a**/2 apart. Each sheet includes Te atoms belonging to the two Te sites. In this case, however, the octahedra do not have the same orientation within one sheet.

Pure sheets of SO_4 tetrahedra are observed as well: they intercalate between the above-described TeO_6 sheets.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36638 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Interatomic distances and angles*

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

(*a*) Te(1) octahedron

Te(1)	O(11)	O(12)	O(13)
O(11)	1·912 (6)	2·694 (9)	2·724 (10)
O(12)	89·1 (3)	1·928 (7)	2·702 (11)
O(13)	90·2 (3)	88·8 (4)	1·934 (7)

(*b*) Te(2) octahedron

Te(2)	O(21)	O(22)	O(23)
O(21)	1·941 (6)	2·655 (12)	2·836 (17)
O(22)	87·9 (4)	1·885 (9)	2·791 (16)
O(23)	94·1 (4)	94·0 (6)	1·932 (12)

(*c*) SO_4 tetrahedron

S	O(1)	O(2)	O(3)	O(4)
O(1)	1·437 (7)	2·397 (10)	2·368 (10)	2·373 (10)
O(2)	113·1 (5)	1·436 (7)	2·353 (10)	2·339 (10)
O(3)	109·4 (5)	108·5 (4)	1·464 (7)	2·382 (11)
O(4)	109·6 (5)	107·4 (5)	108·8 (5)	1·467 (8)

(*d*) Environment of Tl(1) and Tl(2)

$Tl(1^{iv})$—$O(1^{i})$	3·026 (8)	$Tl(2^{i})$—$O(1^{ii})$	3·163 (8)
$Tl(1^{iv})$—$O(2^{ii})$	3·197 (7)	$Tl(2^{i})$—$O(2^{iv})$	3·031 (8)
$Tl(1^{iv})$—$O(12^{i})$	3·126 (9)	$Tl(2^{i})$—$O(11^{ii})$	2·971 (7)
$Tl(1^{iv})$—$O(13^{ii})$	2·888 (8)	$Tl(2^{i})$—$O(12^{ii})$	2·906 (7)
$Tl(1^{iv})$—$O(21^{i})$	3·109 (7)	$Tl(2^{i})$—$O(13^{iv})$	3·057 (8)
$Tl(1^{iv})$—$O(22^{i})$	3·274 (11)	$Tl(2^{i})$—$O(21^{ii})$	2·880 (7)
$Tl(1^{iv})$—$O(22^{ii})$	2·809 (11)	$Tl(2^{i})$—$O(23^{iv})$	3·249 (14)
$Tl(1^{iv})$—$O(23^{ii})$	2·937 (9)		

Symmetry code

The Arabic numerals, (1) through (4), (11) through (13) and (21) through (23) correspond to crystallographically independent atoms. The Roman numerals correspond to the positions given in the *Introduction*.

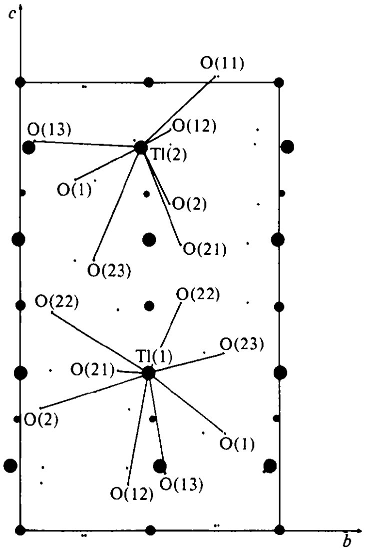

Fig. 3. Projection of $Te(OH)_6.Tl_2SO_4$ along the *a* axis emphasizing the environment of Tl(1) and Tl(2). The positions represented correspond to those indicated in Table 2(*d*).

The structure also shows mixed sheets – of $Te(OH)_6$ octahedra and SO_4 tetrahedra – parallel to (010).

There is a small difference between the environments of Tl(1) and Tl(2), as can be seen in Table 2 and Fig. 3. Tl(1) has eight neighbors, whereas Tl(2) has only seven. In both cases the distances are such that $2{\cdot}8 < Tl{-}O < 3{\cdot}3$ Å. The environment of Tl(1) is made up of two O atoms belonging to two different SO_4 tetrahedra, two O atoms belonging to the same TeO_6 octahedron corresponding to Te(1), two O atoms belonging to the same TeO_6 octahedron corresponding to Te(2) and two O atoms belonging to two different TeO_6 octahedra corresponding to the equivalent Te(2).

The environment of Tl(2) is made up of two O atoms belonging to two different SO_4 tetrahedra, three O atoms belonging to TeO_6 octahedra corresponding to Te(1) and two O atoms belonging to one TeO_6 octahedron corresponding to Te(2).

No attempt has been made to locate the protons of the hydrogen bonds in this structure.

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