

Dipotassium selenate tellurate

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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{Se}-\text{O}) = 0.002$ Å
 R factor = 0.019
 wR factor = 0.021
Data-to-parameter ratio = 11.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

This work is a correction of our earlier structural study where the structure of $\text{K}_2\text{SeO}_4\text{Te}(\text{OH})_6$ (KSeTe) was published in the non-centrosymmetric space group Cc [Dammak *et al.* (1999). *J. Solid State Chem.* **145**, 612–618]. The present X-ray structure determination, using remeasured intensities, shows that KSeTe is monoclinic in space group $C2/c$. In this structure, the Te atom lies on a centre of symmetry and the Se atom on a twofold axis.

Comment

In a previous paper, we reported that potassium selenate tellurate, $\text{K}_2\text{SeO}_4\text{Te}(\text{OH})_6$ (KSeTe), crystallizes in the non-centrosymmetric space group Cc (Dammak *et al.*, 1999). Dielectric and physical studies made thereafter on this compound (Dammak *et al.*, 2000) showed that the space group at room temperature must be centrosymmetric. Here, we correct the previous structure. In the present study, we have assumed that $\text{K}_2\text{SeO}_4\text{Te}(\text{OH})_6$ crystallizes in the monoclinic space group $C2/c$. The structure was studied by X-ray diffraction using a remeasured diffraction pattern.

The structure is built of layers of TeO_6 octahedra at $z = 0$ and $z = c/2$, separated by layers of SeO_4 tetrahedra perpendicular to the c axis at $z = c/4$ and $z = 3c/4$. The K^+ cation is intercalated between the two kinds of layers. In the KSeTe structure, the Te atom, occupying a special position lying on a centre of symmetry, has an octahedral coordination formed by six O atoms. The TeO_6 octahedra are more regular than those in the potassium sulfate tellurate compound (Zilber *et al.*, 1980), where the Te–O distances are between 1.914 and 1.938 Å, with O–Te–O angles varying from 89.3 to 90.5°. In the earlier KSeTe structure determination, the Te–O distances varied from 1.867 (7) to 1.946 (7) Å. In consequence, the octahedral groups are more regular in the present report than in the earlier report (Dammak *et al.*, 1999).

The Se atom, located on a twofold axis, has a tetrahedral environment composed of four O atoms. The selenate tetrahedra were more distorted in the Cc structure than in the correct $C2/c$ structure.

In contrast with potassium sulfate tellurate, where the environment of the K atom is octahedral (Zilber *et al.*, 1980), and with the earlier report of the KSeTe structure (Dammak *et al.*, 1999), where it is coordinated by nine O atoms, the K^+ cation in the present potassium selenate tellurate structure is coordinated by seven O atoms. Each cation is coordinated by three O atoms belonging to SeO_4 tetrahedra and four O atoms belonging to $\text{Te}(\text{OH})_6$ octahedra.

The $\text{K}_2\text{SeO}_4\text{Te}(\text{OH})_6$ structure is stabilized by hydrogen bonds formed with all the H atoms belonging to the $\text{Te}(\text{OH})_6$ octahedra. Three bonds link the SeO_4 tetrahedra and the TeO_6

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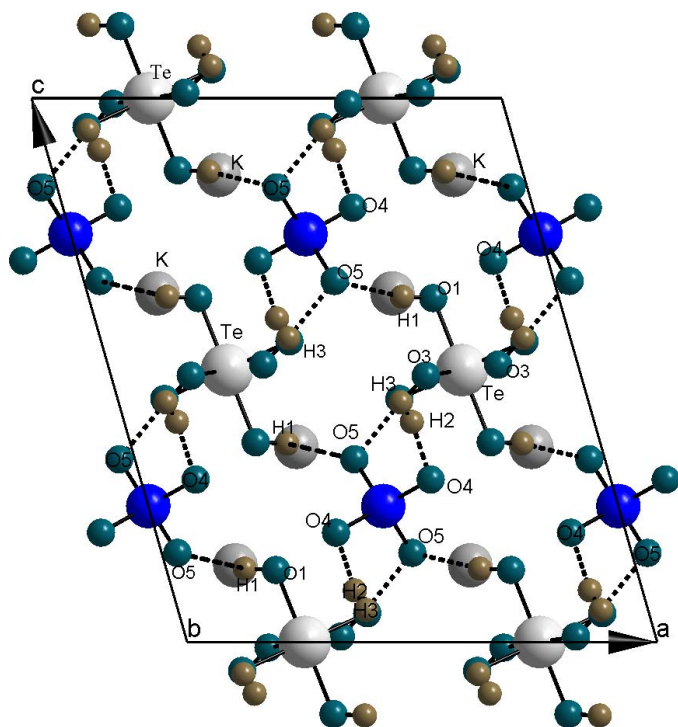


Figure 1
The crystal structure of $K_2SeO_4Te(OH)_6$, showing the hydrogen bonds (dashed lines).

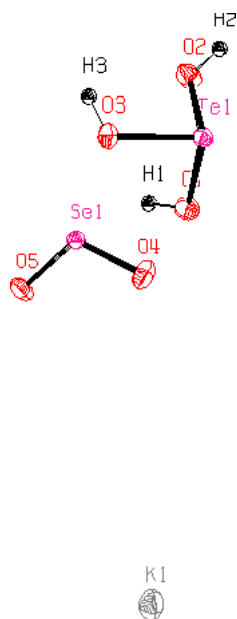


Figure 2
A displacement ellipsoid plot of $K_2SeO_4Te(OH)_6$, with ellipsoids at the 50% probability level.

octahedra. In consequence, in the SeO_4 tetrahedra, one O atom (O5) participates in the establishment of two hydrogen bonds, whereas atom O4 is linked to only one H atom. Fig. 1 shows the structural arrangement of the $KSeTe$ material with hydrogen bonds. The projection of the structure shows the presence of a chain parallel to the $[101]$ direction connected by the third ($O5 \cdots H1$) hydrogen bond.

Experimental

Single crystals of $K_2SeO_4Te(OH)_6$ were synthesized by slow evaporation at room temperature of an aqueous solution of telluric acid (H_6TeO_6) and potassium selenate (K_2SeO_4) in a stoichiometric ratio, as described in our previous work (Dammak *et al.*, 1999).

Crystal data

$K_2SeO_4Te(OH)_6$
 $M_r = 450.81$
 Monoclinic, $C2/c$
 $a = 11.536$ (2) Å
 $b = 6.427$ (1) Å
 $c = 13.898$ (3) Å
 $\beta = 105.95$ (3)°
 $V = 990.8$ (3) Å³
 $Z = 4$

$D_x = 3.022$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 3431 reflections
 $\theta = 2-25^\circ$
 $\mu = 7.55$ mm⁻¹
 $T = 293$ K
 Prism, white
 $0.10 \times 0.05 \times 0.05$ mm

Data collection

Nonius KappaCCD diffractometer
 φ scans
 Absorption correction: multi-scan (*MULABS* in *PLATON*; Spek, 2003)
 $T_{min} = 0.641$, $T_{max} = 0.680$
 3431 measured reflections

918 independent reflections
 883 reflections with $I > 3\sigma(I)$
 $R_{int} = 0.042$
 $\theta_{max} = 25.7^\circ$
 $h = -13 \rightarrow 13$
 $k = -7 \rightarrow 7$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F
 $R = 0.019$
 $wR = 0.021$
 $S = 1.04$
 883 reflections
 79 parameters
 All H-atom parameters refined
 Robust weighting:
 $w = [1 - (F_o - F_c)^2/36\sigma^2(F_o)]^2 / [1.85T_o(x) - 0.632T_1(x)]$

+ $1.4T_2(x)$],
 where $x = F_o/F_{max}$ and $T_i(x)$ are Chebyshev polynomials (Prince, 1982)
 $(\Delta/\sigma)_{max} = 0.002$
 $\Delta\rho_{max} = 0.87$ e Å⁻³
 $\Delta\rho_{min} = -0.56$ e Å⁻³
 Extinction correction: Larson (1970), equation 22
 Extinction coefficient: 87 (3)

Table 1

Selected geometric parameters (Å, °).

Te1—O1	1.9195 (18)	K1—O1 ⁱ	2.849 (2)
Te1—O2	1.9131 (18)	K1—O2 ⁱⁱ	2.847 (2)
Te1—O3	1.9141 (17)	K1—O3 ⁱⁱⁱ	2.8580 (18)
Se1—O4	1.6322 (18)	K1—O4 ^{iv}	2.794 (2)
Se1—O5	1.6416 (16)	K1—O5 ^v	2.7775 (19)
O1—Te1—O2	89.55 (8)	O2 ^{vi} —Te1—O3	89.15 (8)
O1 ^{vi} —Te1—O2	90.45 (8)	O4—Se1—O4 ^{vii}	109.47 (15)
O1—Te1—O3	89.89 (8)	O4—Se1—O5	110.84 (9)
O1 ^{vi} —Te1—O3	90.11 (8)	O4 ^{viii} —Se1—O5	107.36 (9)
O2—Te1—O3	90.85 (8)		

Symmetry codes: (i) $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$; (ii) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$; (iii) $\frac{1}{2} + x, \frac{3}{2} - y, \frac{1}{2} + z$; (iv) $1 - x, 1 - y, 1 - z$; (v) $\frac{1}{2} - x, \frac{3}{2} - y, 1 - z$; (vi) $\frac{1}{2} - x, \frac{1}{2} - y, -z$; (vii) $-x, y, \frac{1}{2} - z$.

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H1 \cdots O5 ^{vii}	0.85 (4)	1.98 (4)	2.824 (3)	170 (4)
O2—H2 \cdots O4 ^{viii}	0.84 (4)	1.83 (4)	2.668 (3)	171 (3)
O3—H3 \cdots O5 ^{ix}	0.90 (4)	1.84 (4)	2.724 (3)	169 (4)

Symmetry codes: (vii) $-x, y, \frac{1}{2} - z$; (viii) $x, -y, z - \frac{1}{2}$; (ix) $x, 1 - y, z - \frac{1}{2}$.

H atoms were located in an electron-density difference map and were refined isotropically.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *CRYSTALS*.

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