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$K_2(SO_4)_{0.63}(SeO_4)_{0.37}\cdot Te(OH)_6$

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Key indicators: single-crystal X-ray study; T = 298 K; mean σ(e–O) = 0.007 Å; disorder in main residue; R factor = 0.045; wR factor = 0.051; data-to-parameter ratio = 15.1.

The title compound, dipotassium sulfate selenate/telluric acid adduct, $K_2(SO_4)_{0.63}(SeO_4)_{0.47}\cdot Te(OH)_6$, is a solid solution in the series $K_2SO_4\cdot Te(OH)_6/K_2SeO_4\cdot Te(OH)_6$. It crystallizes in the same structure as the end member $K_2SO_4\cdot Te(OH)_6$ in the space group $P\overline{1}$, whereas the other end-member $K_2SeO_4\cdot Te(OH)_6$ crystallizes in the space group $C2/c$. The structure of the solid solution consists of planes of $Te(OH)_6$ octahedra alternating with planes of statistically occupied XO_4 tetrahedra (X = S and Se), and with K^+ cations situated between the planes. The structure is stabilized by interplanar O—H···O hydrogen bonds involving all the H atoms that belong to the OH groups of the $Te(OH)_6$ octahedra. Both Te atoms lie on inversion centres.

Related literature

For the structures of the end-members of this solid solution series, see $K_2SO_4\cdot Te(OH)_6$ (Zilber *et al.*, 1980) and $K_2SeO_4\cdot Te(OH)_6$ (Dammak *et al.*, 2005).

Experimental

Crystal data

$K_2(SO_4)_{0.63}(SeO_4)_{0.37}Te(OH)_6$
M_r = 421.16
Triclinic, $P\overline{1}$
a = 6.2463 (2) Å
b = 6.6470 (2) Å
c = 13.1326 (4) Å
α = 102.138 (2)°
β = 90.073 (2)°
γ = 116.943 (1)°
V = 472.28 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 5.63 mm^{-1}
T = 298 K
0.15 × 0.14 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*MULABS* in *PLATON*; Spek, 2003)
T_{min} = 0.447, T_{max} = 0.569
69116 measured reflections
2787 independent reflections
1719 reflections with $I > 3\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.051
S = 1.09
1719 reflections
114 parameters
7 restraints
H-atom parameters refined
$\Delta\rho_{max}$ = 2.40 e Å^{-3}
$\Delta\rho_{min}$ = −2.99 e Å^{-3}

Table 1
Selected bond lengths (Å).

X = S and Se.

Te1—O1	1.920 (6)	K1—O6	2.897 (6)
Te1—O2	1.900 (6)	K1—O1	2.984 (7)
Te1—O3	1.915 (6)	K1—O5	2.990 (6)
Te2—O4	1.905 (6)	K1—O8^{v}	3.022 (8)
Te2—O5	1.919 (5)	K1—O10^{v}	3.032 (8)
Te2—O6	1.921 (6)	K2—O10^{v}	2.709 (6)
X1—O7	1.508 (6)	K2—O2^{i}	2.751 (6)
X1—O8	1.460 (7)	K2—O8^{vi}	2.786 (8)
X1—O9	1.482 (7)	K2—O9^{vii}	2.852 (7)
X1—O10	1.473 (6)	K2—O1^{v}	2.908 (7)
K1—O4^{iii}	2.792 (6)	K2—O3^{vii}	2.915 (6)
K1—O7	2.815 (6)	K2—O6	2.984 (7)
K1—O5^{iv}	2.889 (6)	K2—O3^{viii}	3.267 (8)

Symmetry codes: (i) $-x, -y, -z$; (iii) $x-1, y, z$; (iv) $-x+1, -y+1, -z+1$; (v) $x+1, y, z$; (vi) $x+1, y-1, z$; (vii) $x, y-1, z$; (viii) $-x+1, -y, -z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O9^{vii}	0.857 (6)	1.924 (7)	2.780 (9)	175.6 (5)
O2—H2···O9	0.817 (6)	1.967 (7)	2.773 (10)	168.7 (5)
O3—H3···O10^{v}	0.817 (6)	1.972 (7)	2.778 (9)	169.1 (5)
O4—H4···O8^{vi}	0.848 (6)	1.815 (7)	2.654 (9)	169.7 (5)
O5—H5···O7^{v}	0.856 (6)	1.868 (6)	2.701 (9)	164.3 (4)
O6—H6···O7^{vii}	0.826 (6)	1.946 (6)	2.755 (8)	166.0 (5)

Symmetry codes: (v) $x+1, y, z$; (vi) $x+1, y-1, z$; (vii) $x, y-1, z$.

Data collection: *COLLECT* (Nonius, 2001); cell refinement: *DENZO*/*SCALEPACK*; data reduction: *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2119).

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supplementary materials

Acta Cryst. (2007). E**63**, i153-i154 [**doi:10.1107/S1600536807027705**]

$K_2(SO_4)_{0.63}(SeO_4)_{0.37}\cdot Te(OH)_6$

M. Abdelhedi, L. Ktari, M. Dammak, A. Cousson and **A. Kolsi**

Comment

Fig. 1 shows a projection of the title structure (I) on the *ab* plane. The structure consists of planes of $Te(OH)_6$ octahedra alternating with planes of statistically occupied XO_4 tetrahedra (X = S, Se). The $Te(OH)_6$ layers extend parallel to the *ac* plane at $y = 0$, whereas the parallel XO_4 layers are at $y \simeq 0.5$. The K^+ cations are situated between the layers.

The two independent Te atoms in (I) occupy inversion centres (Fig. 2), with very similar Te—O distances between 1.900 (6) and 1.921 (6) Å and O—Te—O angles between 88.8 (3) and 91.20 (3)°. In the isostructural end-member $K_2SO_4\cdot Te(OH)_6$ (KSTe) (Zilber *et al.*, 1980), the Te—O distances are nearly the same and vary from 1.914 (5) to 1.938 (5) Å, whilst in $K_2SeO_4\cdot Te(OH)_6$ (KSeTe) they are between 1.913 (2) and 1.919 (2) Å (Dammak *et al.*, 2005).

The X—O distances of the slightly distorted XO_4 tetrahedra vary from 1.460 (7) to 1.508 (6) Å, with O—X—O angles between 108.3 (4) and 111.0 (4)°. In the KSTe structure, the S—O distances range from 1.453 (5) to 1.503 (5) Å and in the KSeTe homologue, the Se—O distances vary from 1.627 (7) to 1.659 (7) Å.

The two K^+ cations are both in eightfold coordination with distances ranging between 2.709 (6) and 3.267 (8) Å. $K1^+$ is coordinated by three O atoms belonging to two XO_4 tetrahedra, by one O atom of a $Te1O_6$ octahedron, and by four O atoms of three $Te2O_6$ octahedra. The environment of $K2^+$ consists of three O atoms belonging to three XO_4 tetrahedra, of one O atom from a $Te2O_6$ octahedron, and of four O atoms from three $Te1O_6$ octahedra.

Interplanar O—H···O hydrogen bonding between the $Te(OH)_6$ octahedra and the XO_4 tetrahedra helps to consolidate the structural set-up. In consequence, all H atoms of the hydroxyl groups participate in the formation of hydrogen bonding. In the XO_4 group, two oxygen atoms are acceptors of one H atom, whereas the other O atoms are acceptors of two H atoms. The O···O distances vary from 2.654 (9) to 2.780 (9) Å and the O—H···O angles range from 164.3 (4) and 175.6 (5)° (Table 1, Fig. 3).

Experimental

Transparent, colorless single crystals of compound (I) were grown at room temperature by slow evaporation of an aqueous solution consisting of a mixture of $Te(OH)_6$ (Aldrich, 99%), K_2SeO_4 (Aldrich, 99.99%) and K_2SO_4 (Aldrich, 99%) in the stoichiometric ratio 1:0.5:0.5.

Refinement

Hydrogen atoms on $Te(OH)_6$ groups were located in a difference map and were refined with restrained distances between 0.81 (1) and 0.86 (1) Å and a common U_{iso} parameter. For the refinement of the occupation factors for S and Se, their sum was constrained to be equal to 1. The highest peak and the deepest hole in the final Fourier map are located 0.04 and 0.57 Å, respectively, from the *X* site (*X* = S, Se).

Figures

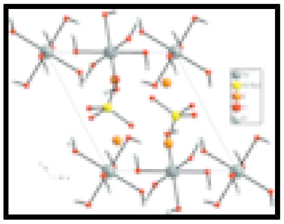

Fig. 1. Projection of the $K_2(SO_4)_{0.63}(SeO_4)_{0.37}\cdot Te(OH)_6$ crystal structure on the *ab* plane.

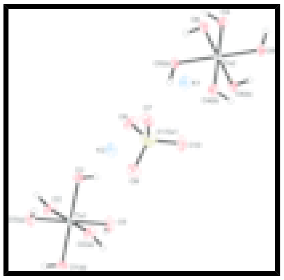

Fig. 2. The asymmetric unit of $K_2(SO_4)_{0.63}(SeO_4)_{0.37}\cdot Te(OH)_6$ (expanded by symmetry to give complete $Te(OH)_6$ octahedra) with displacement ellipsoids drawn at the 50% probability level. [Symmetry codes:(*a*) −*x*, −*y*, −*z*; (*b*) −*x* + 1, −*y*, −*z* + 1].

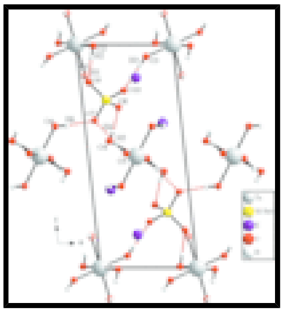

Fig. 3. The hydrogen bonding (dotted lines) in the crystal structure of $K_2(SO_4)_{0.63}(SeO_4)_{0.37}\cdot Te(OH)_6$.

Dipotassium sulfate/selenate tellurate

Crystal data

$K_2(SO_4)_{0.63}(SeO_4)_{0.37}Te(OH)_6$	$Z = 2$
$M_r = 421.16$	$F_{000} = 397.250$
Triclinic, $P\overline{1}$	$D_x = 2.961$ Mg m^{-3}
Hall symbol: -P 1	Mo *K*α radiation λ = 0.71073 Å
a = 6.2463 (2) Å	Cell parameters from 7138 reflections
b = 6.6470 (2) Å	θ = 2.7–30.1°
c = 13.1326 (4) Å	μ = 5.63 mm^{-1}
α = 102.138 (2)°	*T* = 298 K
β = 90.073 (2)°	Prism, colourless
γ = 116.943 (1)°	0.15 × 0.14 × 0.10 mm
V = 472.28 (3) Å^3	

Data collection

Nonius KappaCCD diffractometer

Monochromator: graphite

$T = 298$ K

φ rotation scans with 2° width

Absorption correction: multi-scan (MULABS in PLATON; Spek, 2003)

$T_{\min} = 0.447$, $T_{\max} = 0.569$

69116 measured reflections

2787 independent reflections

1719 reflections with $I > 3\sigma(I)$

$R_{\text{int}} = 0.038$

$\theta_{\max} = 30.2°$

$\theta_{\min} = 1.6°$

$h = -8\rightarrow8$

$k = -9\rightarrow9$

$l = -18\rightarrow18$

Refinement

Refinement on F

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.051$

$S = 1.09$

1719 reflections

114 parameters

7 restraints

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

All H-atom parameters refined

Method, part 1, Chebychev polynomial, [Watkin (1994). Acta Cryst. A50, 411–437; Prince, (1982). Mathematical Techniques in Crystallography and Materials Science. Springer-Verlag: New York.] [weight] = $1.0/[A_0*T_0(x) + A_1*T_1(x) \cdots + A_{n-1}]*T_{n-1}(x)]$ where A_i are the Chebychev coefficients listed below and x = F/Fmax Method = Robust Weighting (Prince, 1982) W = [weight] * $[1-(\text{delta}F/6*\text{sigma}F)^2]^2$ A_i are: 4.11 -3.38 2.64

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 2.40$ e Å^{-3}

$\Delta\rho_{\min} = -2.99$ e Å^{-3}

Extinction correction: None

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{\text{iso}}*/U_{\text{eq}}$	Occ. (<1)
Te1	0.0000	0.0000	0.0000	0.0150	
Te2	0.5000	0.0000	0.5000	0.0144	
Se1	−0.24991 (17)	0.46625 (17)	0.24814 (17)	0.0439	0.368 (7)
S1	−0.24991 (17)	0.46625 (17)	0.24814 (17)	0.0439	0.632 (7)
K1	0.1921 (4)	0.2576 (3)	0.35079 (18)	0.0274	
K2	0.4207 (4)	−0.2342 (3)	0.14873 (17)	0.0254	
O1	−0.0604 (11)	−0.0373 (10)	0.1399 (5)	0.0232	
O2	−0.1770 (12)	0.1704 (11)	0.0061 (5)	0.0251	
O3	0.2905 (11)	0.2817 (10)	0.0548 (6)	0.0269	
O4	0.7680 (10)	−0.0037 (10)	0.4321 (5)	0.0250	
O5	0.6055 (11)	0.3137 (9)	0.4891 (5)	0.0215	

O6	0.3083 (10)	−0.1107 (10)	0.3668 (5)	0.0233
O7	−0.1044 (11)	0.4714 (11)	0.3412 (5)	0.0260
O8	−0.3641 (13)	0.6150 (12)	0.2807 (6)	0.0281
O9	−0.0842 (12)	0.5509 (12)	0.1687 (6)	0.0312
O10	−0.4411 (12)	0.2270 (10)	0.2057 (6)	0.0301
H1	−0.0693	−0.1671	0.1452	0.0436*
H2	−0.1419	0.2746	0.0589	0.0436*
H3	0.3657	0.2491	0.0937	0.0436*
H4	0.7229	−0.1343	0.3896	0.0436*
H5	0.6985	0.3395	0.4404	0.0436*
H6	0.1875	−0.2315	0.3702	0.0436*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Te1	0.01489 (9)	0.01533 (9)	0.01406 (9)	0.00653 (9)	0.00131 (9)	0.00335 (9)
Te2	0.01472 (9)	0.01349 (9)	0.01512 (9)	0.00649 (9)	0.00155 (9)	0.00350 (9)
Se1	0.03752 (17)	0.04897 (17)	0.03836 (17)	0.01470 (17)	0.00249 (17)	0.00931 (17)
S1	0.03752 (17)	0.04897 (17)	0.03836 (17)	0.01470 (17)	0.00249 (17)	0.00931 (17)
K1	0.0242 (8)	0.0260 (8)	0.0370 (11)	0.0156 (7)	0.0043 (7)	0.0079 (7)
K2	0.0244 (8)	0.0227 (8)	0.0346 (10)	0.0146 (7)	0.0013 (7)	0.0093 (7)
O1	0.033 (3)	0.025 (3)	0.016 (3)	0.015 (2)	0.007 (2)	0.009 (2)
O2	0.031 (3)	0.028 (3)	0.024 (3)	0.022 (3)	0.000 (2)	0.003 (2)
O3	0.025 (3)	0.016 (2)	0.035 (4)	0.004 (2)	−0.007 (2)	0.008 (2)
O4	0.019 (3)	0.020 (3)	0.032 (3)	0.008 (2)	0.008 (2)	0.001 (2)
O5	0.026 (3)	0.013 (2)	0.026 (3)	0.009 (2)	0.006 (2)	0.006 (2)
O6	0.024 (3)	0.019 (3)	0.020 (3)	0.004 (2)	−0.004 (2)	0.006 (2)
O7	0.023 (3)	0.031 (3)	0.028 (3)	0.011 (2)	0.000 (2)	0.017 (3)
O8	0.036 (4)	0.032 (3)	0.029 (4)	0.029 (3)	0.006 (3)	0.001 (3)
O9	0.032 (3)	0.030 (3)	0.033 (4)	0.013 (3)	0.006 (3)	0.012 (3)
O10	0.031 (3)	0.016 (3)	0.038 (4)	0.007 (2)	−0.005 (3)	0.005 (2)

Geometric parameters (Å, °)

Te1—O1^{i}	1.920 (6)	O4—H4	0.848
Te1—O3^{i}	1.915 (6)	O5—H5	0.856
Te1—O2^{i}	1.900 (6)	O6—H6	0.826
Te1—O1	1.920 (6)	K1—O4^{iii}	2.792 (6)
Te1—O2	1.900 (6)	K1—O7	2.815 (6)
Te1—O3	1.915 (6)	K1—O5^{iv}	2.889 (6)
Te2—O6^{ii}	1.921 (6)	K1—O6	2.897 (6)
Te2—O5^{ii}	1.919 (5)	K1—O1	2.984 (7)
Te2—O4^{ii}	1.905 (6)	K1—O5	2.990 (6)
Te2—O4	1.905 (6)	K1—O8^{v}	3.022 (8)
Te2—O5	1.919 (5)	K1—O10^{v}	3.032 (8)
Te2—O6	1.921 (6)	K2—O10^{v}	2.709 (6)

X1—O7	1.508 (6)	K2—O2^{i}	2.751 (6)
X1—O8	1.460 (7)	K2—O8^{vi}	2.786 (8)
X1—O9	1.482 (7)	K2—O9^{vii}	2.852 (7)
X1—O10	1.473 (6)	K2—O1^{v}	2.908 (7)
O1—H1	0.857	K2—O3^{vii}	2.915 (6)
O2—H2	0.817	K2—O6	2.984 (7)
O3—H3	0.817	K2—O3^{viii}	3.267 (8)
O1^{i}—Te1—O3^{i}	89.9 (3)	O6^{ii}—Te2—O5	90.4 (3)
O1^{i}—Te1—O2^{i}	91.2 (3)	O5^{ii}—Te2—O5	179.994
O3^{i}—Te1—O2^{i}	90.4 (3)	O4^{ii}—Te2—O5	90.0 (3)
O1^{i}—Te1—O1	179.994	O4—Te2—O5	90.0 (3)
O3^{i}—Te1—O1	90.1 (3)	O6^{ii}—Te2—O6	179.994
O2^{i}—Te1—O1	88.8 (3)	O5^{ii}—Te2—O6	90.4 (3)
O1^{i}—Te1—O2	88.8 (3)	O4^{ii}—Te2—O6	89.6 (3)
O3^{i}—Te1—O2	89.6 (3)	O4—Te2—O6	90.4 (3)
O2^{i}—Te1—O2	179.994	O5—Te2—O6	89.6 (3)
O1—Te1—O2	91.2 (3)	O7—X1—O8	109.8 (4)
O1^{i}—Te1—O3	90.1 (3)	O7—X1—O9	108.3 (4)
O3^{i}—Te1—O3	179.994	O8—X1—O9	110.1 (4)
O2^{i}—Te1—O3	89.6 (3)	O7—X1—O10	109.3 (4)
O1—Te1—O3	89.9 (3)	O8—X1—O10	108.4 (4)
O2—Te1—O3	90.4 (3)	O9—X1—O10	111.0 (4)
O6^{ii}—Te2—O5^{ii}	89.6 (3)	Te1—O1—H1	109.426
O6^{ii}—Te2—O4^{ii}	90.4 (3)	Te1—O2—H2	114.986
O5^{ii}—Te2—O4^{ii}	90.0 (3)	Te1—O3—H3	105.734
O6^{ii}—Te2—O4	89.6 (3)	Te2—O4—H4	109.438
O5^{ii}—Te2—O4	90.0 (3)	Te2—O5—H5	108.396
O4^{ii}—Te2—O4	179.994	Te2—O6—H6	106.016

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x+1, -y, -z+1$; (iii) $x-1, y, z$; (iv) $-x+1, -y+1, -z+1$; (v) $x+1, y, z$; (vi) $x+1, y-1, z$; (vii) $x, y-1, z$; (viii) $-x+1, -y, -z$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O9^{vii}	0.857 (6)	1.924 (7)	2.780 (9)	175.6 (5)
O2—H2···O9	0.817 (6)	1.967 (7)	2.773 (10)	168.7 (5)
O3—H3···O10^{v}	0.817 (6)	1.972 (7)	2.778 (9)	169.1 (5)
O4—H4···O8^{vi}	0.848 (6)	1.815 (7)	2.654 (9)	169.7 (5)
O5—H5···O7^{v}	0.856 (6)	1.868 (6)	2.701 (9)	164.3 (4)
O6—H6···O7^{vii}	0.826 (6)	1.946 (6)	2.755 (8)	166.0 (5)

Symmetry codes: (vii) $x, y-1, z$; (v) $x+1, y, z$; (vi) $x+1, y-1, z$.

Fig. 1

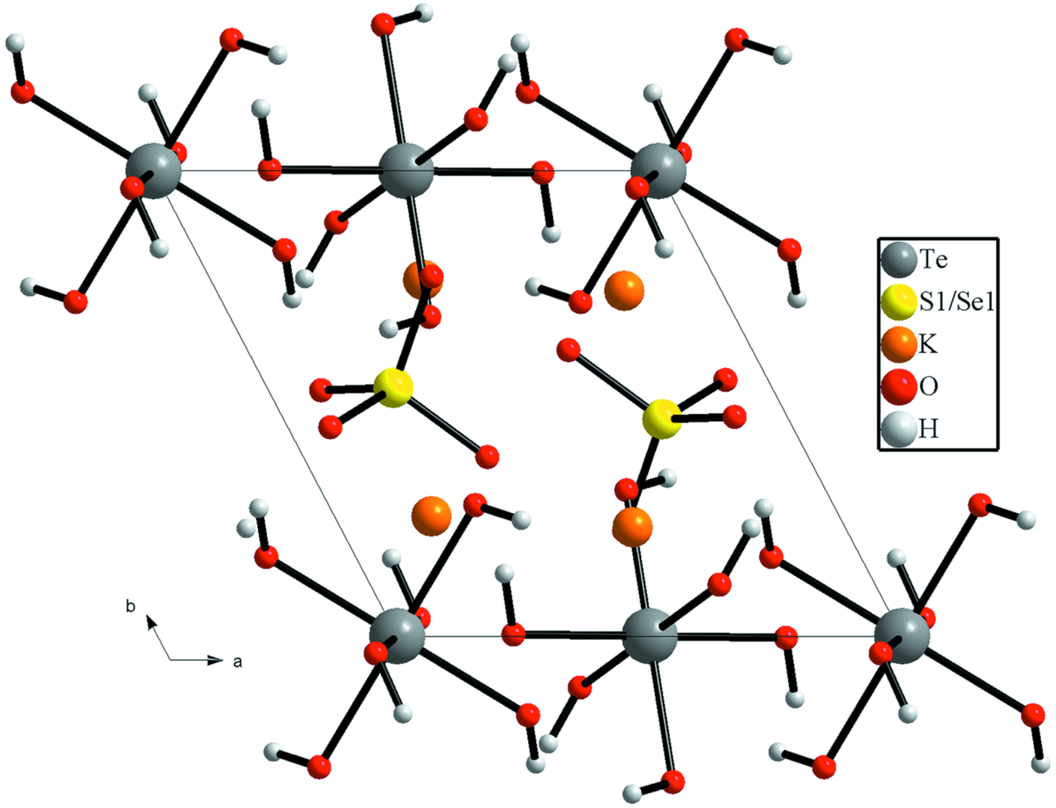

Fig. 2

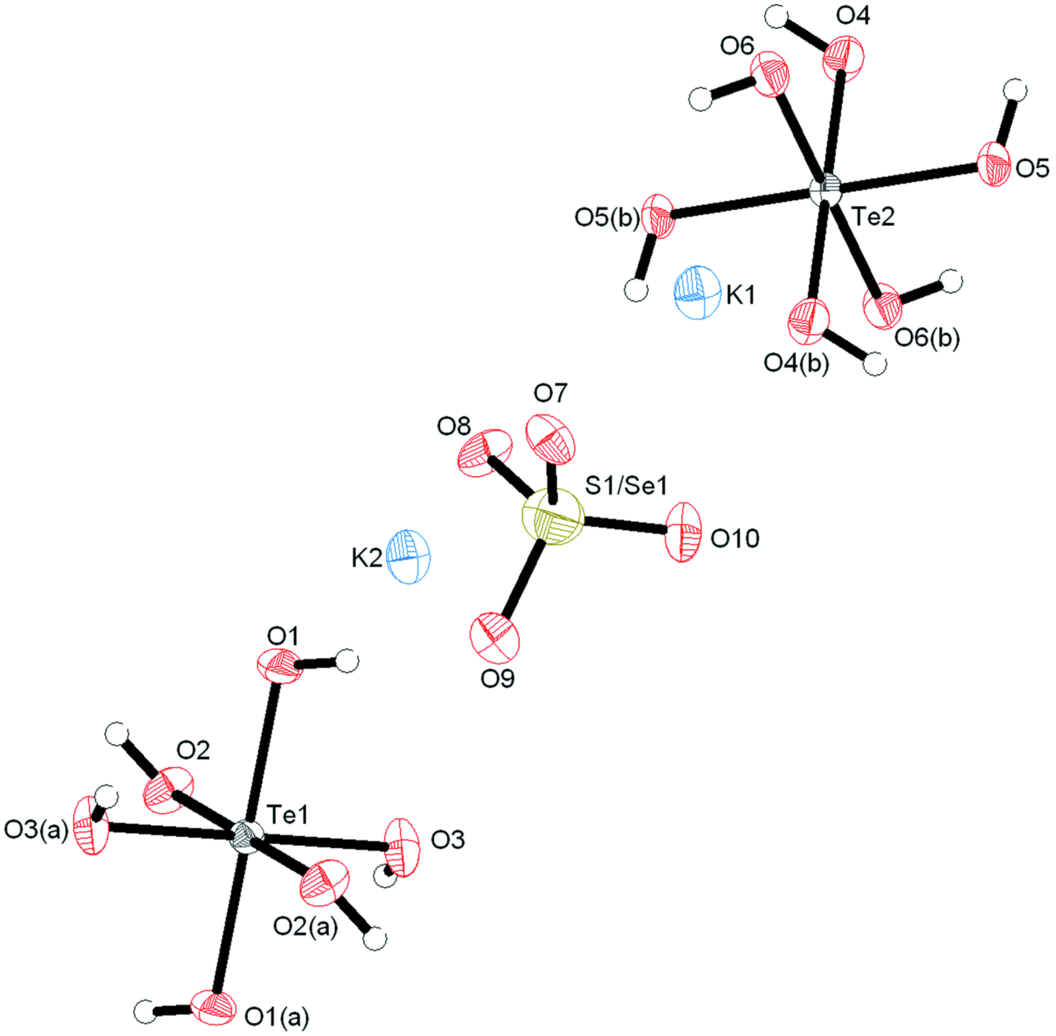
O4
O6
O5
O5(b)
Te2
K1
O6(b)
O4(b)
O7
O8
S1/Se1
O10
K2
O9
O1
O2
Te1
O3(a)
O3
O2(a)
O1(a)

Fig. 3