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$(NH_4)_2(SO_4)_{0.71}(SeO_4)_{0.29}Te(OH)_6$

Mohamed Abdelhedi,[a,b]* Mohamed Dammak,[b] Alain Cousson,[a] Marrot Jérome[c] and Kolsi Abdelwaheb[b]

[a]Laboratoire Léon Brillouin, CE/Saclay, Bâtiment 563, 91191 Gif-sur-Yvette Cedex, France, [b]Laboratoire de l'Etat Solide, Faculté des Sciences de Sfax, 3018 Sfax, Tunisia, and [c]Institut Lavoisier de Versailles, UMR 8180, Université de Versailles, 45 Avenue des Etats Unis, 78035 Versailles, France
Correspondence e-mail: m_abdelhedi2002@yahoo.fr

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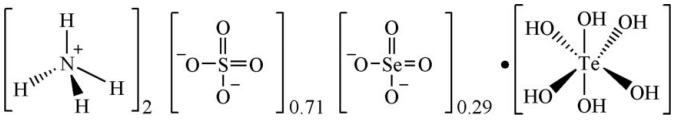
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(S–O) = 0.0012 Å; R factor = 0.016; wR factor = 0.021; data-to-parameter ratio = 19.4.

The main feature of the title structure, ammonium sulfate selenate tellurate, is the presence of three different chalcogenate species in the same compound. The crystal structure contains planes of SO_4/SeO_4 tetrahedra alternating with planes of $Te(OH)_6$ octahedra. Disordered NH_4^+ cations are intercalated between these planes. Both octahedra and SO_4/SeO_4 tetrahedra are linked by O—H···O hydrogen bonds.

Related literature

For related literature, see: Abdelhedi, Dammak, Cousson, Nierlich & Kolsi (2005); Abdelhedi, Dammak, Cousson & Kolsi (2005); Litaiem *et al.* (2005); Zilber *et al.* (1981).



Experimental

Crystal data

$(NH_4)_2(SO_4)_{0.71}(SeO_4)_{0.29}Te(OH)_6$
M_r = 385.23
Monoclinic, $P2_1/c$
a = 13.7340 (2) Å
b = 6.6583 (1) Å
c = 11.4582 (2) Å
β = 106.827 (1)°
V = 1002.93 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.20 mm^{-1}
T = 298 K
0.30 × 0.26 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*MULABS* in *PLATON*; Spek, 2003)
T_{min} = 0.32, T_{max} = 0.43
14354 measured reflections
2940 independent reflections
2213 reflections with $I > 3\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.021
S = 1.01
2213 reflections
114 parameters
1 restraint
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Data collection: *COLLECT* (Nonius, 2001); cell refinement: *DENZO/SCALEPACK*; data reduction: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS86* (Sheldrick, 1986); 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: PK2023).

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supplementary materials

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$(NH_4)_2(SO_4)_{0.71}(SeO_4)_{0.29}Te(OH)_6$

M. Abdelhedi, M. Dammak, A. Cousson, M. Jérome and K. Abdelwaheb

Comment

In pursuing our study of sulfate selenate tellurate salts, amongst which we have solved $Cs_2(SO_4)_{0.57}(SeO_4)_{0.43}\cdot Te(OH)_6$ (Abdelhedi, Dammak, Cousson, Nierlich & Abdelwaheb, 2005) and $Rb_2(SO_4)_{0.5}(SeO_4)_{0.5}\cdot Te(OH)_6$ (Abdelhedi, Dammak, Cousson & Kolsi, 2005), we have grown the title compound, $(NH_4)_2(SO_4)_{0.71}(SeO_4)_{0.29}\cdot Te(OH)_6$ (NSSeTe). The structure (Fig. 1) is built up of planes of $Te(OH)_6$ octahedra (at x = 0 and 1/2) alternating with planes of SO_4/SeO_4 tetrahedra (at x = 1/4 and 3/4), with disordered NH_4 cations intercalated between these planes. The S and Se atoms occupy the same site. In the SO_4/SeO_4 tetrahedra, the S/Se—O distances range from 1.5165 (12) Å to 1.5246 (12) Å, intermediate between those in $(NH_4)_2SO_4\cdot Te(OH)_6$ (1.373 (11)–1.565 (8) Å) (Zilber *et al.*, 1981) and $(NH_4)_2SeO_4\cdot Te(OH)_6$ (1.622 (4)–1.639 (4) Å) (Litaiem *et al.*, 2005). In the octahedral groups, the Te—O distances vary from 1.9021 (13) to 1.9133 (11) Å with O—Te—O angles that range between 87.15 (5) and 92.85 (5)°. Each NH_4 cation is coordinated to three oxygen atoms belonging to S/SeO_4 tetrahedra and six oxygen atoms from $Te(OH)_6$ octahedra. The structure is stabilized by O—H···O hydrogen bonds. The O···H distances in this compound vary from 1.7558 (12)Å to 1.897 (11)Å with O—H···O angles ranging from 155.47 (8)° to 172.90 (11)°. Figure 2 shows the packing arrangement of the NSSeTe material.

Experimental

Transparent, colorless single crystals of the title composition were grown from aqueous solution of a mixture of telluric acid, H_6TeO_6 (Aldrich, 99%), ammonium carbonate $(NH_4)_2CO_3$, (Aldrich 99.9%), selenic acid, H_2SeO_4 (Aldrich 94%) and ammonium sulfate $(NH_4)_2SO_4$, (Aldrich 99.999%) at room temperature. (The stoichiometric ratio 1:0.5:0.5:0.5).

Refinement

Hydrogen atoms on $Te(OH)_6$ groups were located in an electron density difference map and were refined isotropically. As a result of disorder, ammonium hydrogen atoms could not be found and therefore could not be included in the model.

Figures

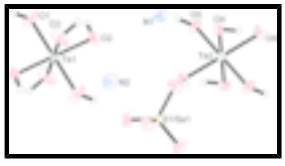


Fig. 1. A part of the structure of $(NH_4)_2(SO_4)_{0.71}(SeO_4)_{0.29}Te(OH)_6$, showing the asymmetric unit (expanded by symmetry to give complete tellurate octahedra). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes:(*a*) −*x* + 1,-*y*, −*z*; b) −*x*, −*y* + 1, −*z*]

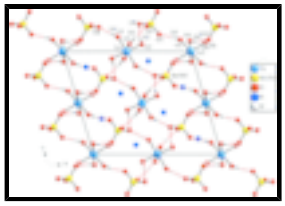


Fig. 2. Crystal structure of $(NH_4)_2(SO_4)_{0.71}(SeO_4)_{0.29}Te(OH)_6$ showing the hydrogen bonds.

Diammonium sulfate-selenate tellurate

Crystal data

$2(NH_4)^+ \cdot O_4S_{0.71}Se_{0.29}^{2-} \cdot H_6O_6Te$	F_{000} = 724.66
M_r = 385.23	D_x = 2.552 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 7138 reflections
a = 13.7340 (2) Å	θ = 2.7–30.1°
b = 6.6583 (1) Å	μ = 4.20 mm^{-1}
c = 11.4582 (2) Å	T = 298 K
β = 106.827 (1)°	Parallelepiped, colourless
V = 1002.93 (3) Å^3	0.30 × 0.26 × 0.20 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	2213 reflections with $I > 3\sigma(I)$
Monochromator: graphite	R_{int} = 0.030
T = 298 K	θ_{max} = 30.1°
φ rotation scans with 2°steps	θ_{min} = 3.1°
Absorption correction: multi-scan (MULABS in PLATON; Spek, 1998)	h = −19→19
T_{min} = 0.32, T_{max} = 0.43	k = −8→9
14354 measured reflections	l = −16→16
2940 independent reflections	

Refinement

Refinement on F	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	All H-atom parameters refined
	Method, part 1, Chebychev polynomial, (Watkin, 1994, *P*rince, 1982) [*w*eight] = 1.0/[A_0*T_0(x) + A_1*T_1(x) ··· + A_{n-1}]*T_{n-1}(x)] where A_i are the Chebychev coefficients listed below and x = F /Fmax Method = Robust Weighting (*P*rince, 1982) W = [*w*eight] * [1-(delta$F$/6*sigma$F$)^2]^2 A_i are: 0.466 0.314 0.278
$R[F^2 > 2\sigma(F^2)]$ = 0.016	

	*P*rince, E. (1982). *Mathematical Techniques in Crystallography and Materials Science*. Springer-Verlag: Ne*w* York. Watkin, D. (1994). *Acta Cryst.* A**50**, 411–437.
$wR(F^2) = 0.021$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.64$ e Å^{-3}
2213 reflections	$\Delta\rho_{min} = -0.42$ e Å^{-3}
114 parameters	Extinction correction: Larson 1970 Crystallographic Computing eq 22
1 restraint	Extinction coefficient: 22.5 (17)
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Te1	0.5000	0.0000	0.0000	0.0154	
Te2	0.0000	0.5000	0.0000	0.0147	
Se1	0.248690 (13)	−0.010650 (13)	0.233850 (13)	0.0152	0.2869 (11)
S1	0.248690 (13)	−0.010650 (13)	0.233850 (13)	0.0152	0.7131 (11)
N1	0.14479 (12)	0.4841 (2)	0.34630 (14)	0.0278	
N2	0.35360 (14)	0.4953 (2)	0.09225 (17)	0.0352	
O1	0.46433 (12)	−0.0932 (2)	0.13912 (13)	0.0452	
O2	0.63403 (8)	−0.10532 (19)	0.06867 (11)	0.0283	
O3	0.53678 (11)	0.25802 (19)	0.07172 (13)	0.0401	
O4	0.01747 (9)	0.73221 (17)	0.10219 (11)	0.0261	
O5	−0.05209 (9)	0.35904 (17)	0.11395 (11)	0.0268	
O6	0.13448 (8)	0.41154 (18)	0.08537 (11)	0.0246	
O7	0.20637 (10)	0.0546 (2)	0.33679 (12)	0.0331	
O8	0.33787 (9)	0.12668 (18)	0.23575 (11)	0.0285	
O9	0.28331 (10)	−0.22762 (18)	0.25249 (11)	0.0318	
O10	0.16707 (10)	0.00918 (17)	0.11171 (11)	0.0311	
H1	0.4196	−0.0021	0.1629	0.0380*	
H2	0.6289	−0.2126	0.1214	0.0450*	
H3	0.6021	0.2640	0.1280	0.0470*	
H4	0.0737	0.7940	0.0949	0.0470*	
H5	−0.0969	0.4446	0.1410	0.0440*	
H6	0.1315	0.2718	0.1009	0.0550*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Te1	0.013986 (18)	0.015896 (18)	0.016686 (18)	0.001266 (18)	0.004796 (18)	0.000916 (18)
Te2	0.015036 (18)	0.015496 (18)	0.014246 (18)	−0.000284 (18)	0.005266 (18)	0.000376 (18)
Se1	0.014780 (13)	0.015480 (13)	0.015440 (13)	−0.001180 (13)	0.004510 (13)	−0.000510 (13)
S1	0.014780 (13)	0.015480 (13)	0.015440 (13)	−0.001180 (13)	0.004510 (13)	−0.000510 (13)
N1	0.0320 (7)	0.0270 (7)	0.0255 (6)	0.0011 (5)	0.0100 (6)	−0.0006 (5)
N2	0.0403 (9)	0.0311 (8)	0.0371 (8)	−0.0007 (6)	0.0158 (7)	−0.0002 (6)
O1	0.0571 (9)	0.0488 (8)	0.0440 (8)	0.0286 (7)	0.0374 (7)	0.0248 (7)

O2	0.0180 (5)	0.0303 (6)	0.0351 (6)	0.0045 (5)	0.0053 (4)	0.0070 (5)
O3	0.0372 (7)	0.0227 (6)	0.0469 (8)	0.0033 (5)	−0.0092 (6)	−0.0090 (5)
O4	0.0263 (5)	0.0244 (5)	0.0293 (5)	−0.0038 (4)	0.0109 (4)	−0.0098 (4)
O5	0.0324 (6)	0.0246 (5)	0.0295 (6)	0.0026 (5)	0.0187 (5)	0.0077 (4)
O6	0.0184 (5)	0.0256 (5)	0.0272 (5)	0.0021 (4)	0.0025 (4)	0.0013 (4)
O7	0.0347 (6)	0.0374 (6)	0.0337 (6)	−0.0065 (5)	0.0199 (5)	−0.0074 (5)
O8	0.0280 (6)	0.0287 (6)	0.0320 (6)	−0.0055 (5)	0.0135 (5)	−0.0047 (4)
O9	0.0306 (6)	0.0244 (6)	0.0360 (6)	0.0017 (5)	0.0028 (5)	0.0016 (5)
O10	0.0319 (6)	0.0267 (6)	0.0288 (6)	−0.0039 (5)	−0.0005 (4)	0.0018 (4)

Geometric parameters (Å, °)

Te1—O2^{i}	1.9133 (11)	Se1—O8	1.5236 (12)
Te1—O3^{i}	1.9083 (12)	Se1—O9	1.5165 (12)
Te1—O1^{i}	1.9021 (13)	Se1—O10	1.5246 (12)
Te1—O1	1.9021 (13)	S1—O7	1.5213 (12)
Te1—O2	1.9133 (11)	S1—O8	1.5236 (12)
Te1—O3	1.9083 (12)	S1—O9	1.5165 (12)
Te2—O6^{ii}	1.9154 (10)	S1—O10	1.5246 (12)
Te2—O4^{ii}	1.9122 (11)	O1—H1	0.957
Te2—O5^{ii}	1.9075 (11)	O2—H2	0.951
Te2—O4	1.9122 (11)	O3—H3	0.942
Te2—O5	1.9075 (11)	O4—H4	0.900
Te2—O6	1.9154 (10)	O5—H5	0.954
Se1—O7	1.5213 (12)	O6—H6	0.950
O2^{i}—Te1—O3^{i}	92.85 (5)	O4—Te2—O5	89.09 (5)
O2^{i}—Te1—O1^{i}	89.22 (6)	O6^{ii}—Te2—O6	179.994
O3^{i}—Te1—O1^{i}	91.89 (7)	O4^{ii}—Te2—O6	89.75 (5)
O2^{i}—Te1—O1	90.78 (6)	O5^{ii}—Te2—O6	90.21 (5)
O3^{i}—Te1—O1	88.11 (7)	O4—Te2—O6	90.25 (5)
O1^{i}—Te1—O1	179.994	O5—Te2—O6	89.79 (5)
O2^{i}—Te1—O2	179.994	O7—Se1—O8	107.68 (7)
O3^{i}—Te1—O2	87.15 (5)	O7—Se1—O9	109.71 (8)
O1^{i}—Te1—O2	90.78 (6)	O8—Se1—O9	110.59 (7)
O1—Te1—O2	89.22 (6)	O7—Se1—O10	110.04 (8)
O2^{i}—Te1—O3	87.15 (5)	O8—Se1—O10	109.60 (7)
O3^{i}—Te1—O3	179.994	O9—Se1—O10	109.21 (6)
O1^{i}—Te1—O3	88.11 (7)	O7—S1—O8	107.68 (7)
O1—Te1—O3	91.89 (7)	O7—S1—O9	109.71 (8)
O2—Te1—O3	92.85 (5)	O8—S1—O9	110.59 (7)
O6^{ii}—Te2—O4^{ii}	90.25 (5)	O7—S1—O10	110.04 (8)
O6^{ii}—Te2—O5^{ii}	89.79 (5)	O8—S1—O10	109.60 (7)
O4^{ii}—Te2—O5^{ii}	89.09 (5)	O9—S1—O10	109.21 (6)
O6^{ii}—Te2—O4	89.75 (5)	Te1—O1—H1	111.974

O4^{ii}—Te2—O4	179.994	Te1—O2—H2	107.281
O5^{ii}—Te2—O4	90.91 (5)	Te1—O3—H3	114.442
O6^{ii}—Te2—O5	90.21 (5)	Te2—O4—H4	105.768
O4^{ii}—Te2—O5	90.91 (5)	Te2—O5—H5	109.488
O5^{ii}—Te2—O5	179.994	Te2—O6—H6	108.017

Symmetry codes: (i) −*x*+1, −*y*, −*z*; (ii) −*x*, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*—H···*A*
O1—H1···O8	0.9572 (13)	1.7984 (12)	166.50 (9)
O2—H2···O8^{iii}	0.9512 (12)	1.8974 (11)	158.11 (8)
O3—H3···O9^{iv}	0.9420 (13)	1.7628 (12)	172.90 (11)
O4—H4···O10^{v}	0.9000 (11)	1.8951 (12)	155.47 (8)
O5—H5···O7^{vi}	0.9538 (12)	1.7558 (12)	162.99 (9)
O6—H6···O10	0.9504 (12)	1.8101 (12)	158.93 (8)

Symmetry codes: (iii) −*x*+1, *y*−1/2, −*z*+1/2; (iv) −*x*+1, *y*+1/2, −*z*+1/2; (v) *x*, *y*+1, *z*; (vi) −*x*, *y*+1/2, −*z*+1/2.

Fig. 1

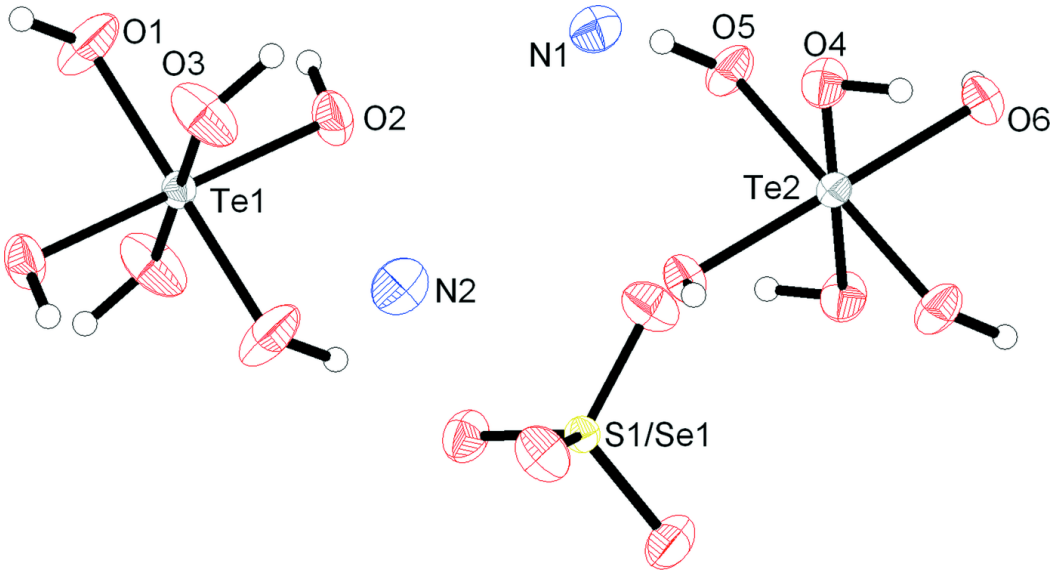
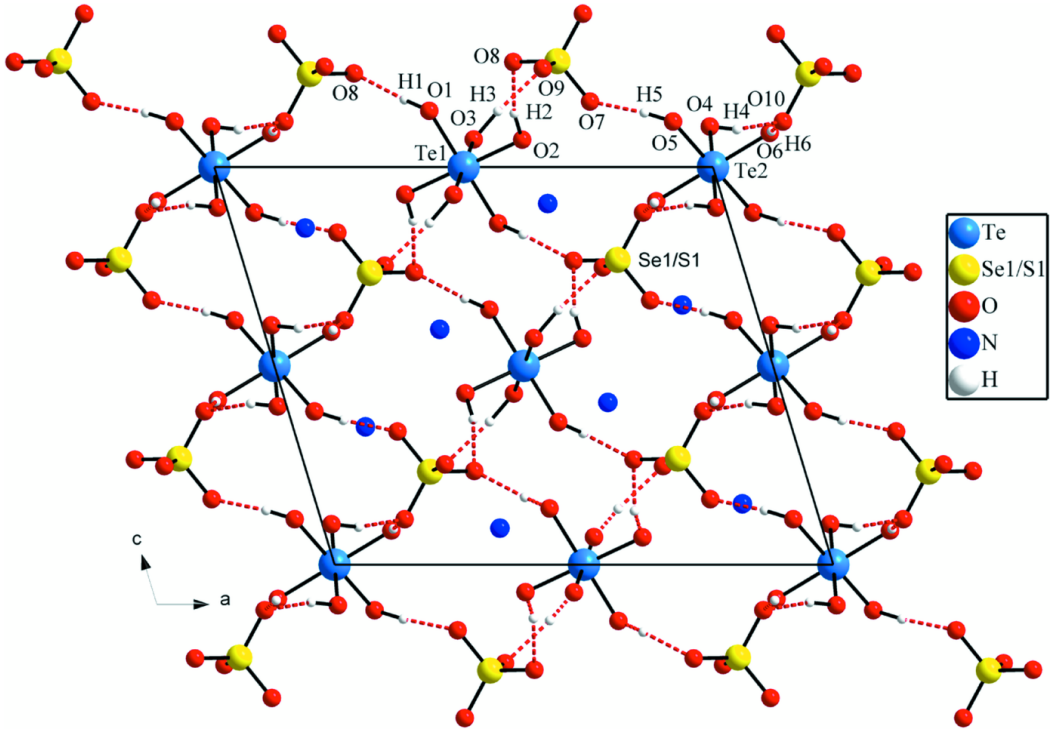


Fig. 2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H1
O1
O8
H3
O9
H5
O4
H4
O10
O3
H2
O7
O5
O6
H6
Te1
O2
Te2
Se1/S1
Te
Se1/S1
O
N
H
c
a