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Y_2TeO_6 with the La_2TeO_6-type structure

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Y–O) = 0.004 Å
R factor = 0.019
wR factor = 0.045
Data-to-parameter ratio = 13.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Of rare-earth metal hexaoxotellurates(VI), only the structures of formula type RE_2TeO_6 are known so far. Diyttrium(III) hexaoxotellurate(VI), Y_2TeO_6, crystallizes isotypically with the orthorhombic La_2TeO_6-prototype structure in space group $P2_12_12_1$. Single crystals were obtained by fusing a mixture of Y_2O_3 and TeO_3 (1:1 molar ratio) in evacuated silica ampoules. The crystal structure is built up by alternating zigzag chains of edge-sharing [$Y1O_7$] and vertex-sharing [$Y2O_7$] polyhedra. Both chain types are arranged in interpenetrating tetragonal rod-packings and are joined to each other by sharing common edges and vertices. The three-dimensional $[Y_2O_6]^{6-}$ framework has channels along [100] in which the Te^{6+} cations reside, leading to discrete [TeO_6] octahedra.

Comment

Y_2TeO_6 is isotypic with rare-earth metal(III) hexaoxotellurates(VI) of the orthorhombic La_2TeO_6 type (RE = Ce–Nd, Sm–Tm) (Nathanson, 1968; Hützler *et al.*, 1984; Trömel *et al.*, 1987; Meier & Schleid, 2003; Meier & Schleid, 2004; Höss & Schleid, 2007*a*), except for the heaviest rare-earth metals Yb and Lu (Nathanson, 1968; Malone *et al.*, 1969; Hützler *et al.*, 1984; Trömel *et al.*, 1987; Höss *et al.*, 2007) and further for

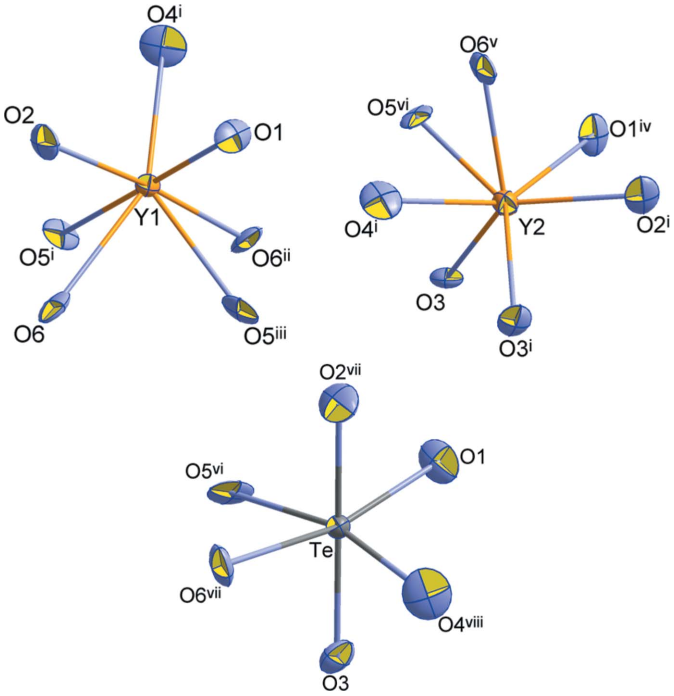

Figure 1
The oxygen coordination environment about $(Y1)^{3+}$, $(Y2)^{3+}$ and Te^{6+}. Displacement ellipsoids are drawn at the 95% probability level. Symmetry codes are as in Table 1.

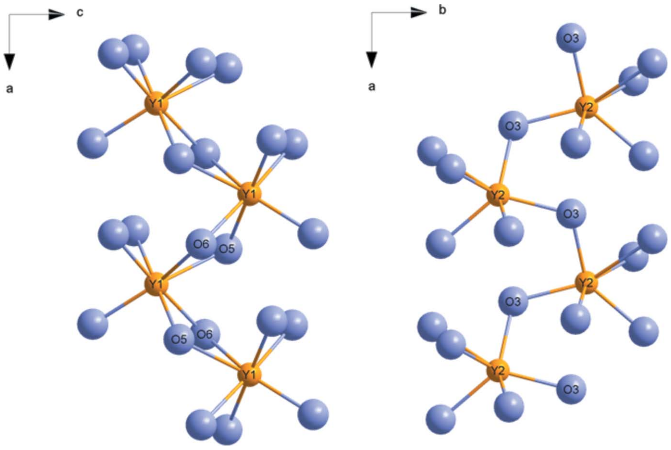

Figure 2
Zigzag chains of edge-sharing [Y1O$_7$] and vertex-connected [Y2O$_7$] polyhedra running along [100].

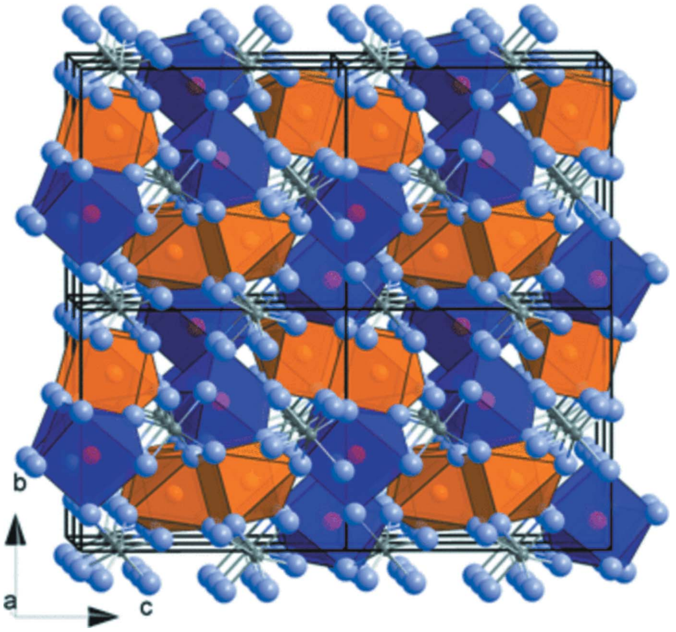

Figure 3
The crystal structure of Y$_2$TeO$_6$ projected approximately along [$\bar{1}$00]. The [Y1O$_7$] polyhedra are shown in orange and the [Y2O$_7$] polyhedra in purple. O and Te atoms are represented as light-blue and grey spheres, respectively.

Sc (Höss & Schleid, 2007*b*), which all adopt the trigonal Na$_2$SiF$_6$-type structure (Zalkin *et al.*, 1964).

The structure of the title compound contains two crystallographically independent Y cations that are both sevenfold coordinated by O atoms (Fig. 1 and Table 1). Both types of yttrium–oxygen polyhedra are condensed to chains in which the [Y1O$_7$] polyhedra are joined by sharing edges (O5–O6) whilst the [Y2O$_7$] polyhedra share common vertices (O3) with each other. Both chain types propagate along [100] and each is arranged independently in the form of a distorted tetragonal rod-packing (O'Keeffe & Andersson, 1977). These two kinds of rod-packings interpenetrate and are further linked by common edges and vertices. The resulting three-dimensional [Y$_2$O$_6$]$^{6-}$ framework has channels in which the Te^{6+} cations reside (Fig. 3). This leads to an octahedral oxygen coordination environment for the unique tellurium cation site (Fig. 1 and Table 1).

The motifs of mutual adjunction (Hoppe, 1980) and coordination numbers (CN) are given in Table 2. Since there are no contacts between the [TeO$_6$] polyhedra, discrete octahedra exist within the structure (Fig. 3), and hence the formula of Y$_2$TeO$_6$ can also be written as Y$_2$[TeO$_6$]. This is in good agreement with the structure descriptions of $M^{\rm I}_6$[TeO$_6$], *e.g.* Li$_6$[TeO$_6$] (Hauck, 1969; Wisser & Hoppe, 1989), and $M^{\rm II}_3$[TeO$_6$] compounds, *e.g.* Ca$_3$[TeO$_6$] (Hottentot & Loopstra, 1981), where isolated [TeO$_6$] octahedra are also present in the structures.

Experimental

Single crystals of Y$_2$TeO$_6$ were obtained from mixtures of the binary oxides Y$_2$O$_3$ and TeO$_3$ in a 1:1 molar ratio. The reaction took place in torch-sealed evacuated silica ampoules at 1073 K for 8 d with a surplus of CsCl as fluxing agent to improve the single-crystal growth. The ampoules were cooled to 773 K within two days, and afterwards the furnace was turned off. The single-phase product Y$_2$TeO$_6$ emerged as block-like colourless and transparent single crystals (approximately 0.2 mm in diameter), which appeared to be stable in air and water.

Crystal data

Y$_2$TeO$_6$
M_r = 401.42
Orthorhombic, $P2_12_12_1$
a = 5.2456 (4) Å
b = 9.0361 (7) Å
c = 9.9312 (8) Å
V = 470.74 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 30.55 mm^{-1}
T = 293 (2) K
0.10 × 0.08 × 0.06 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1999)
$T_{\rm min}$ = 0.043, $T_{\rm max}$ = 0.164
11534 measured reflections
1153 independent reflections
1144 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.088

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.045
S = 1.05
1153 reflections
83 parameters
$\Delta\rho_{\rm max}$ = 0.84 e Å^{-3}
$\Delta\rho_{\rm min}$ = −1.16 e Å^{-3}
Absolute structure: Flack (1983), 454 Friedel pairs
Flack parameter: −0.011 (7)

Table 1
Selected bond lengths (Å).

Y1—O1	2.253 (4)	Y2—O6$^{\rm v}$	2.291 (4)
Y1—O4$^{\rm i}$	2.287 (4)	Y2—O2$^{\rm i}$	2.294 (4)
Y1—O2	2.297 (4)	Y2—O4$^{\rm i}$	2.431 (4)
Y1—O5$^{\rm i}$	2.307 (4)	Y2—O5$^{\rm vi}$	2.591 (4)
Y1—O6$^{\rm ii}$	2.346 (4)	Te—O1	1.893 (4)
Y1—O5$^{\rm iii}$	2.469 (4)	Te—O2$^{\rm vii}$	1.901 (4)
Y1—O6	2.496 (4)	Te—O3	1.909 (4)
Y2—O3	2.215 (4)	Te—O4$^{\rm viii}$	1.922 (4)
Y2—O3$^{\rm i}$	2.258 (3)	Te—O5$^{\rm vi}$	1.938 (4)
Y2—O1$^{\rm iv}$	2.280 (4)	Te—O6$^{\rm vii}$	1.952 (4)

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

Table 2
Motifs of mutual adjunction (Hoppe, 1980) and coordination numbers (CN).

	O1	O2	O3	O4	O5	O6	CN
Y1	1/1	1/1	0/0	1/1	2/2	2/2	7
Y2	1/1	1/1	2/2	1/1	1/1	1/1	7
Te	1/1	1/1	1/1	1/1	1/1	1/1	6
CN	3	3	3	3	4	4	

The deepest hole in the final difference Fourier map is located 0.78 Å from Te.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

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