# inorganic papers

Zn$_3$TeO$_6$

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Key indicators

Single-crystal X-ray study

T = 293 K

Mean σ(Mn–O) = 0.004 Å

R factor = 0.036

wR factor = 0.078

Data-to-parameter ratio = 16.7

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

Single crystals of trizinc(II) hexaoxotellurate(VI), Zn$_3$TeO$_6$, were grown by chemical transport reactions. The compound crystallizes in the β-Li$_3$VF$_6$ structure type and is isotypic with Co$_3$TeO$_6$. It can be derived from a close packing of strongly distorted oxygen layers in an *hhchhc* sequence parallel to (100), with two distinct Te atoms in the octahedral, four Zn atoms in the octahedral and one Zn atom in the tetrahedral interstices. Except for one Te atom and one Zn atom which are located on an inversion centre and on a twofold axis, respectively, all atoms are in general positions.

Comment

Orthotellurates(VI) of the formula type M_3TeO$_6$ (M is a divalent metal) exhibit a rich crystal chemistry. A comparison of the various structure types adopted by M_3TeO$_6$ or $(M,M')_3$TeO$_6$ compounds [in the latter case, the divalent M and M' cations are statistically distributed over the same crystallographic site(s)] is given in the preceding publication (Weil, 2006). We report here the crystal growth and the crystal structure of Zn$_3$TeO$_6$.

Zn$_3$TeO$_6$ crystallizes in the β-Li$_3$VF$_6$ structure type (Massa, 1980) and is isotypic with Co$_3$TeO$_6$ (Becker *et al.*, 2006). The crystal structure of the title compound can be described by a
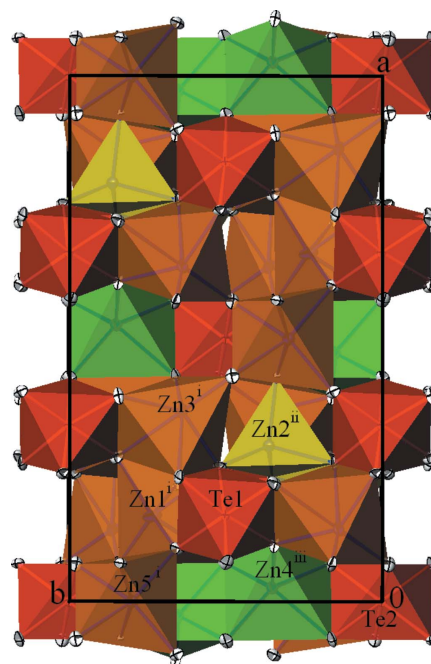
Figure 1

The crystal structure of Zn$_3$TeO$_6$ in polyhedral representation projected along [00$\bar{1}$]. Displacement ellipsoids are drawn at the 74% probability level. [Symmetry codes: (i) x, $1 - y$, $\frac{1}{2} + z$; (ii) $\frac{1}{2} - x$, $\frac{1}{2} - y$, $1 - z$; (iii) $\frac{1}{2} + x$, $\frac{1}{2} - y$, $\frac{1}{2} + z$.]

close packing of distorted oxygen layers in an *hhchhc* sequence parallel to (100) (Becker *et al.*, 2006), with two distinct Te atoms in the octahedral, four Zn atoms in the octahedral and one Zn atom in the tetrahedral interstices. Except for atoms Te2 and Zn5 which are located on an inversion centre and on a twofold axis, respectively, all other atoms are in general positions.

As in all other M_3TeO_6 structures, the TeO_6 octahedra are isolated from each other and show only a slight distortion from ideal geometry, with an average Te—O distance of 1.922 Å (Table 1). The coordination numbers (CN) of the Zn atoms range from 4 to 6. Consistent with its tetrahedral coordination, Zn2 shows the shortest Zn—O distances of all the Zn atoms (Table 1). Atoms Zn1, Zn3 and Zn5 exhibit an octahedral coordination, but with a significant distortion around the first two Zn atoms. Their four closely bonded O atoms have Zn—O separations of about 2.0 Å, whereas the two remaining O atoms augment these polyhedra with Zn—O distances > 2.5 Å, resulting in an overall [4 + 2] coordination. The octahedron around Zn5 is more regular, with an average Zn—O distance of 2.136 Å. Zn4 exhibits CN = 5 and its coordination geometry may be described as square pyramidal with the central Zn atom moved from the basal O atoms towards the apex of the pyramid. The next nearest O atom, *viz.* O3 at $(\frac{1}{2} - x, \frac{1}{2} - y, -z)$, has a distance of 3.178 (4) Å and does not contribute to the first coordination sphere.

By vertex and edge sharing of the TeO_6, ZnO_4, ZnO_5 and ZnO_6 units, the three-dimensional network of the structure is obtained (Fig. 1).

Experimental

Suitable single crystals of Zn_3TeO_6 were grown by chemical transport reactions using Cl_2 as transport agent. Stoichiometric amounts of ZnO and TeO_3 were mixed in the ratio 3:1 and heated together with 50 mg $PtCl_2$ at 1023 K for 30 h in a sealed and evacuated silica ampoule, resulting in a microcrystalline material. The ampoule was then heated in a temperature gradient 1103 → 1023 K. After 5 d, colourless single crystals up to an edge length of 2 mm, mostly with a lath-like habit and sometimes with a plate-like habit, had formed at the colder part of the ampoule. X-ray powder diffraction of the obtained crystals revealed a single phase product.

Crystal data

Zn_3TeO_6	$Z = 12$
$M_r = 419.71$	$D_x = 6.154$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 14.8898 (8)$ Å	$\mu = 22.02$ mm^{-1}
$b = 8.8341 (5)$ Å	$T = 293 (2)$ K
$c = 10.3457 (5)$ Å	Lath, colourless
$\beta = 92.990 (1)°$	$0.18 \times 0.05 \times 0.04$ mm
$V = 1359.00 (12)$ Å^3	

Data collection

Bruker SMART APEX CCD diffractometer	10616 measured reflections
ω scans	2326 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)	2301 reflections with $I > 2\sigma(I)$
$T_{min} = 0.110$, $T_{max} = 0.473$	$R_{int} = 0.029$
(expected range = 0.096–0.414)	$\theta_{max} = 32.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + 46.687P]$
$R[F^2 > 2\sigma(F^2)] = 0.036$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.078$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.44$	$\Delta\rho_{max} = 1.34$ e Å^{-3}
2326 reflections	$\Delta\rho_{min} = -1.70$ e Å^{-3}
139 parameters	Extinction correction: *SHELXL97*
	Extinction coefficient: 0.00100 (5)

Table 1
Selected bond lengths (Å).

Te1—O8^i	1.900 (4)	Zn2—O2	1.967 (4)
Te1—O6^i	1.906 (4)	Zn2—O4^{viii}	1.982 (4)
Te1—O7^i	1.923 (4)	Zn3—O7	1.935 (4)
Te1—O3	1.925 (4)	Zn3—O5	1.976 (4)
Te1—O4	1.927 (4)	Zn3—O1^i	1.986 (5)
Te1—O5	1.943 (4)	Zn3—O9	2.087 (4)
Te2—O1^{ii}	1.904 (4)	Zn3—O4	2.525 (5)
Te2—O1	1.904 (4)	Zn3—O6	2.652 (5)
Te2—O2^{iii}	1.931 (4)	Zn4—O7^{ix}	1.922 (4)
Te2—O2^{iv}	1.931 (4)	Zn4—O8	2.003 (4)
Te2—O9^v	1.932 (4)	Zn4—O8^x	2.014 (4)
Te2—O9^{vi}	1.932 (4)	Zn4—O2^{xi}	2.165 (4)
Zn1—O3	1.938 (4)	Zn4—O9	2.243 (5)
Zn1—O6	1.972 (4)	Zn5—O3^{iii}	2.036 (4)
Zn1—O6^v	2.034 (4)	Zn5—O3	2.036 (4)
Zn1—O9^v	2.081 (4)	Zn5—O1^{iii}	2.162 (5)
Zn1—O5	2.635 (5)	Zn5—O1	2.162 (5)
Zn1—O8^v	2.747 (5)	Zn5—O2^{iii}	2.210 (4)
Zn2—O5^{vii}	1.886 (4)	Zn5—O2	2.210 (4)
Zn2—O4	1.963 (4)		

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

The structural data were standardized using the program *STRUCTURE TIDY* (Gelato & Parthé, 1987). The highest peak in the final Fourier map is 0.86 Å from Te1 and the deepest hole is 0.65 Å from Te1.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ATOMS* (Dowty, 2004); software used to prepare material for publication: *SHELXL97*.

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