

Mn₃TeO₆**Matthias Weil**Institute for Chemical Technologies and
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mweil@mail.zserv.tuwien.ac.at**Key indicators**Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{Mn}-\text{O}) = 0.002 \text{ \AA}$
R factor = 0.014
wR factor = 0.035
Data-to-parameter ratio = 16.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Single crystals of trimanganese(II) hexaoxotellurate(VI), Mn₃TeO₆, were grown by chemical transport reactions. Its structure is isotypic with Mg₃TeO₆ and can be derived from close packing of strongly distorted hexagonal oxygen layers parallel to (001), with Mn and two distinct Te atoms in the octahedral interstices. The TeO₆ octahedra are very regular, with $\bar{3}$ symmetry, whereas the MnO₆ octahedra are considerably distorted.

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Many orthotellurates(VI) of the formula type $(M, M')_3\text{TeO}_6$, where *M* and *M'* are divalent metals, are structurally well characterized. All these structures comprise isolated TeO₆ octahedra and can be divided into six different structure types: Mg₃TeO₆ in the space group $R\bar{3}$, Ni₃TeO₆ (*R*3) as a derivative of corundum, Cu₃TeO₆ ($Ia\bar{3}$) with a bixbyite-type structure, Co₃TeO₆ (*C*2/*c*) with a β -Li₃VF₆-type structure, Ca₃TeO₆ (*P*2₁/*n*) with a cryolite-type structure, and the unique structure of Hg₃TeO₆ ($Ia\bar{3}$). Lattice parameters, space groups, and average Te–O distances of these and related compounds are given in Table 2. The title compound, Mn₃TeO₆, adopts the Mg₃TeO₆ structure type and its crystal structure is reported here.

The atomic arrangement of Mn₃TeO₆ can be derived from close packing of strongly distorted hexagonal oxygen layers parallel to (001), with Mn and two distinct Te atoms in the octahedral interstices (Fig. 1). Both TeO₆ octahedra are isolated and share edges with six MnO₆ octahedra. Each MnO₆ octahedron shares four edges with adjacent MnO₆ octahedra, one edge with a Te1O₆ and another edge with the

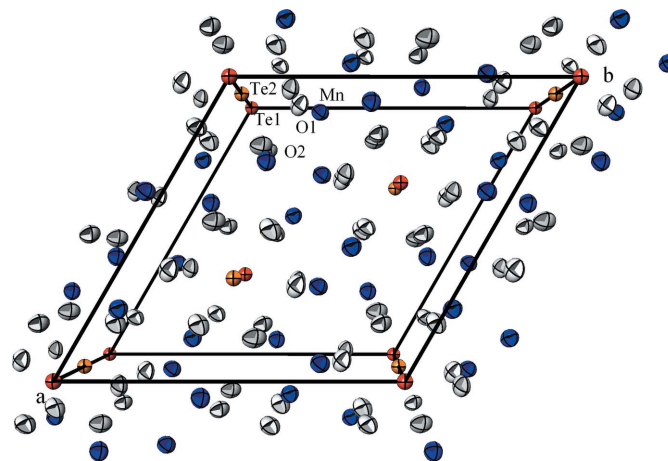


Figure 1
The crystal structure of Mn₃TeO₆ in a perspective view along [00 $\bar{1}$]. Displacement ellipsoids are drawn at the 97% probability level.

TeO₆ octahedron. Each of the two crystallographically independent O atoms is coordinated by one Te and three Mn atoms in a distorted tetrahedral manner. Both TeO₆ octahedra exhibit $\bar{3}$ symmetry and are fairly regular, with an average Te—O distance of 1.923 Å, which is in good agreement with the average Te—O distances of other (M,M')₃TeO₆ compounds (Table 2) and other tellurates(VI) (Levason, 1997). The MnO₆ octahedron is considerably distorted, with distances ranging from 2.1055 (14) to 2.3841 (13) Å (Table 1).

Experimental

A mixture of MnO and TeO₃ in the stoichiometric ratio 3:1 was thoroughly ground, pressed into a pellet and placed in a silica ampoule which was evacuated, sealed, and heated within 3 h to 1103 K and kept at this temperature for 3 d. X-ray powder diffraction of the light-brown microcrystalline material revealed a single phase product. 200 mg of this material was mixed with 50 mg PtCl₂ and loaded in an evacuated and sealed silica ampoule which was heated in a temperature gradient 1103 → 1023 K. At this temperature, PtCl₂ decomposes with release of Cl₂ which then serves as the transport agent. After 5 d, a few amber coloured crystals of the title compound with a plate-like habit and an edge-length up to 0.8 mm had formed in the colder part of the ampoule.

Crystal data

Mn ₃ TeO ₆	$D_x = 5.325 \text{ Mg m}^{-3}$
$M_r = 388.42$	Mo $K\alpha$ radiation
Trigonal, $R\bar{3}$	$\mu = 13.55 \text{ mm}^{-1}$
$a = 8.8673 (10) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 10.6729 (12) \text{ \AA}$	Plate, amber
$V = 726.77 (14) \text{ \AA}^3$	$0.09 \times 0.06 \times 0.02 \text{ mm}$
$Z = 6$	

Data collection

Bruker SMART APEX CCD diffractometer	3003 measured reflections
ω scans	558 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	541 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.375$, $T_{\max} = 0.773$	$R_{\text{int}} = 0.026$
	$\theta_{\max} = 32.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0163P)^2 + 0.5015P]$
$R[F^2 > 2\sigma(F^2)] = 0.014$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.035$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 1.18$	$\Delta\rho_{\max} = 0.59 \text{ e \AA}^{-3}$
558 reflections	$\Delta\rho_{\min} = -1.06 \text{ e \AA}^{-3}$
33 parameters	Extinction correction: <i>SHELXL97</i>
	Extinction coefficient: 0.0116 (3)

Table 1

Selected bond lengths (Å).

Mn—O1	2.1055 (14)	Mn—O2	2.2313 (13)
Mn—O2 ⁱ	2.1275 (13)	Mn—O1 ^{iv}	2.3841 (13)
Mn—O1 ⁱⁱ	2.2009 (13)	Te1—O1	1.9247 (13)
Mn—O2 ⁱⁱⁱ	2.2311 (12)	Te2—O2	1.9214 (12)

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

Table 2

Structural data of (M, M')₃TeO₆ compounds (Å, °), and average Te—O distances (Å).

M,M' ²⁺	space group	a	b	c	β	(Te—O)
Mg ^a	$R\bar{3}$	8.615 (3)		10.315 (3)		1.913
Mn ^b	$R\bar{3}$	8.8673 (10)		10.6729 (12)		1.923
Mn,Cu ^c	$R\bar{3}$	8.826 (1)		10.687 (2)		1.921
Ni ^d	$R\bar{3}$	5.1087 (8)		13.767 (2)		1.940
Cu,Zn ^e	$Ia\bar{3}$	9.537 (1)				1.933
Cu,Co ^f	$Ia\bar{3}$	9.5702 (5)				1.932
Cu,Ni ^g	$Ia\bar{3}$	9.5464 (6)				1.934
Cu ^h	$Ia\bar{3}$	9.5565 (5)				1.921
Co ⁱ	$C2/c$	14.8167 (18)	8.8509 (11)	10.3631 (14)	94.90 (1)	1.932
Zn ^j	$C2/c$	14.8898 (8)	8.8341 (5)	10.3457 (5)	92.990 (1)	1.922
Cu,Zn ^k	$C2/c$	14.834 (2)	8.801 (1)	10.375 (2)	93.27 (2)	1.918
Ca ^l	$P2_1/n$	5.5782 (8)	5.7998 (9)	8.017 (1)	90.217 (5)	1.924
Cd ^l	$P2_1/n$	5.4986 (3)	5.6383 (3)	8.0191 (5)	90.00 (5)	1.925
Hg ^m	$Ia\bar{3}$	13.3808 (6)				1.942

Notes: (a) Schulz & Bayer, 1971; (b) this work; (c) metal ratio: Mn_{2.4}Cu_{0.6}; Wulff et al., 1998; (d) Becker & Berger, 2006; (e) metal ratio: Cu_{1.5}Zn_{1.5}; Wulff & Müller-Buschbaum, 1998; (f) metal ratio: Cu_{1.5}Co_{1.5}; Wulff & Müller-Buschbaum, 1998; (g) metal ratio: Cu₂Ni₁; Wedel et al., 2001; (h) Falck et al., 1978; (i) Becker et al., 2006; (j) Weil, 2006; (k) metal ratio: Cu_{1.667}Zn_{1.333}; Wulff & Müller-Buschbaum, 1998; (l) Burckhardt et al., 1982; (m) Weil, 2003.

The atomic coordinates of Mg₃TeO₆ (Schulz & Bayer, 1971) were taken as starting parameters for the refinement. The structural data were then standardized using the program *STRUCTURE TIDY* (Gelato & Parthé, 1987). The deepest hole in the final Fourier map is 0.61 Å from Te1.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE* (Bruker, 2002); data reduction: *SAINTE*; method used to solve structure: coordinates taken from an isotypic compound; 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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References

- Becker, R. & Berger, H. (2006). *Acta Cryst.* **E62**, i222–i223.
 Becker, R., Johansson, M. & Berger, H. (2006). *Acta Cryst.* **C62**, i67–i69.
 Bruker (2002). *SMART* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Burckhardt, H.-G., Platte, C. & Trömel, M. (1982). *Acta Cryst.* **B38**, 2450–2452.
 Dowty, E. (2004). *ATOMS for Windows*. Version 6.1. Shape Software, Kingsport, Tennessee, USA.
 Falck, L., Lindqvist, O. & Moret, J. (1978). *Acta Cryst.* **B34**, 896–897.
 Gelato, L. M. & Parthé, E. (1987). *J. Appl. Cryst.* **20**, 139–143.
 Levason, W. (1997). *Coord. Chem. Rev.* **161**, 33–79.
 Schulz, H. & Bayer, G. (1971). *Acta Cryst.* **B27**, 815–821.
 Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
 Sheldrick, G. M. (2002). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Wedel, B., Kimio, I. & Sugiyama, K. (2001). *Z. Kristallogr. NCS*, **216**, 323–324.
 Weil, M. (2003). *Z. Anorg. Allg. Chem.* **629**, 653–657.
 Weil, M. (2006). *Acta Cryst.* **E62**, i246–i247.
 Wulff, L. & Müller-Buschbaum, H. (1998). *Z. Naturforsch. Teil B*, **53**, 53–57.
 Wulff, L., Wedel, B. & Müller-Buschbaum, H. (1998). *Z. Naturforsch. Teil B*, **53**, 49–52.