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## Key indicators

Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{Mn}-\text{O}) = 0.002\text{ \AA}$   
 $R$  factor = 0.019  
 $wR$  factor = 0.045  
Data-to-parameter ratio = 22.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Manganese tellurite,  $\beta\text{-MnTe}_2\text{O}_5$ 

Hydrothermally prepared  $\beta\text{-MnTe}_2\text{O}_5$  is isostructural with  $\text{MgTe}_2\text{O}_5$ . It contains infinite layers of corner-sharing  $\text{TeO}_{3+1}$  groups propagating in the  $ac$  plane. Infinite chains of edge-sharing  $\text{MnO}_6$  octahedra [ $d_{\text{av}}(\text{Mn}-\text{O}) = 2.186(2)\text{ \AA}$ ] running along  $[001]$  link the Te/O layers into a continuous structure. Mn and one O atom have site symmetry 2.  $\beta\text{-MnTe}_2\text{O}_5$  complements the known denningite-type phase  $\alpha\text{-MnTe}_2\text{O}_5$ .

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## Comment

$\beta\text{-MnTe}_2\text{O}_5$  is isostructural with  $\text{MgTe}_2\text{O}_5$  (Trömel, 1975). An indexed powder pattern for  $\text{MnTe}_2\text{O}_5$  (which we now call the  $\beta$  modification of this stoichiometry), with a similar orthorhombic cell to that found here, was also given by Trömel, but no further structural details were elucidated.

Synthetic denningite-type  $\text{MnTe}_2\text{O}_5$  (hereafter called  $\alpha\text{-MnTe}_2\text{O}_5$ ) has a completely different structure (Miletich, 1993) containing unusual  $\text{MnO}_8$  groups, as well as very distorted  $\text{MnO}_6$  octahedra and  $\text{TeO}_4$  moieties. The formula of the  $\alpha$  phase is sometimes written as  $\text{Mn}_2(\text{Te}_2\text{O}_5)_2$  to emphasise the different Mn coordinations and an extensive substitution chemistry is possible at both the eight- and six-coordinate metal sites (Walitzi, 1964; Miletich, 1993).  $\beta\text{-MnTe}_2\text{O}_5$  is slightly denser than  $\alpha\text{-MnTe}_2\text{O}_5$  ( $\rho = 5.198\text{ Mg m}^{-3}$ ).

In  $\beta\text{-MnTe}_2\text{O}_5$ , the manganese cation (site symmetry 2) is coordinated by six O atoms in distorted octahedral geometry. The average Mn–O separation of  $2.186(2)\text{ \AA}$  is in good agreement with the ionic radius sum for high-spin  $\text{Mn}^{\text{II}}$  and  $\text{O}^{2-}$  ( $2.19\text{ \AA}$ ; Shannon, 1976). The bond valence sum (BVS) of 2.07, calculated by the Brown formalism (1996), is close to the

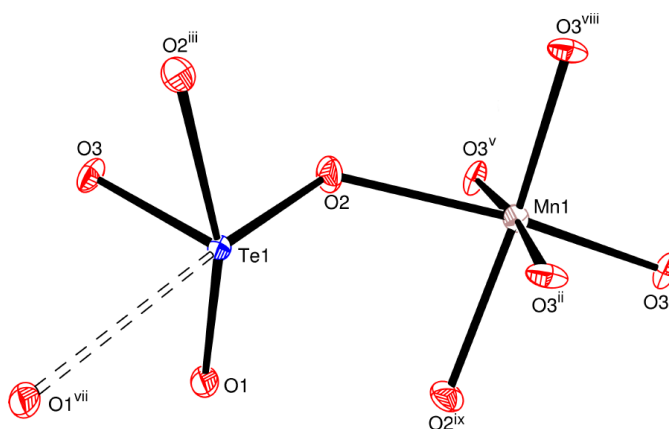
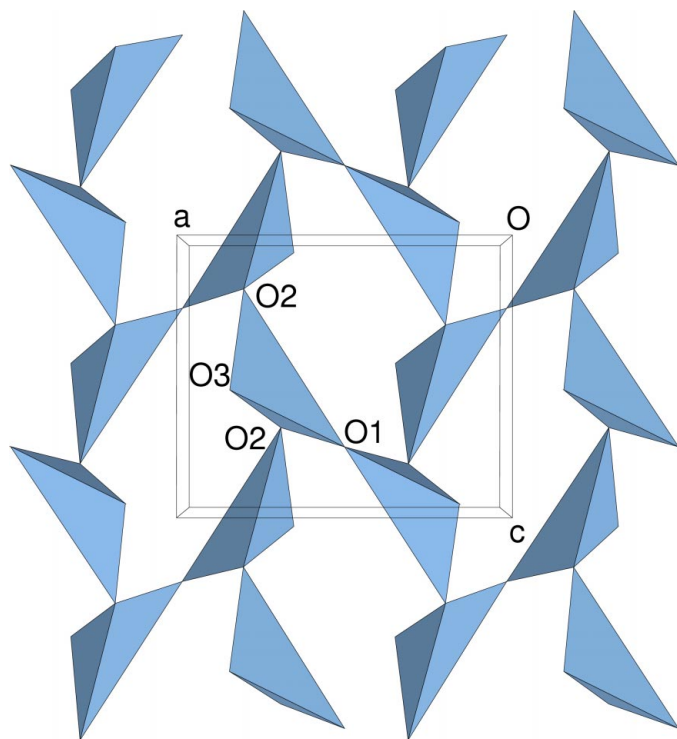


Figure 1

Fragment of  $\beta\text{-MnTe}_2\text{O}_5$  (50% probability displacement ellipsoids), showing the atom connectivity and labelling scheme. The long  $\text{Te1}\cdots\text{O1}^{\text{vii}}$  contact is indicated by a dashed bond. Symmetry codes as in Table 1; additionally, (vii)  $-x, 1-y, 1-z$ ; (viii)  $\frac{1}{2}-x, y-\frac{1}{2}, z$ ; (ix)  $-x, y, \frac{1}{2}-z$ .



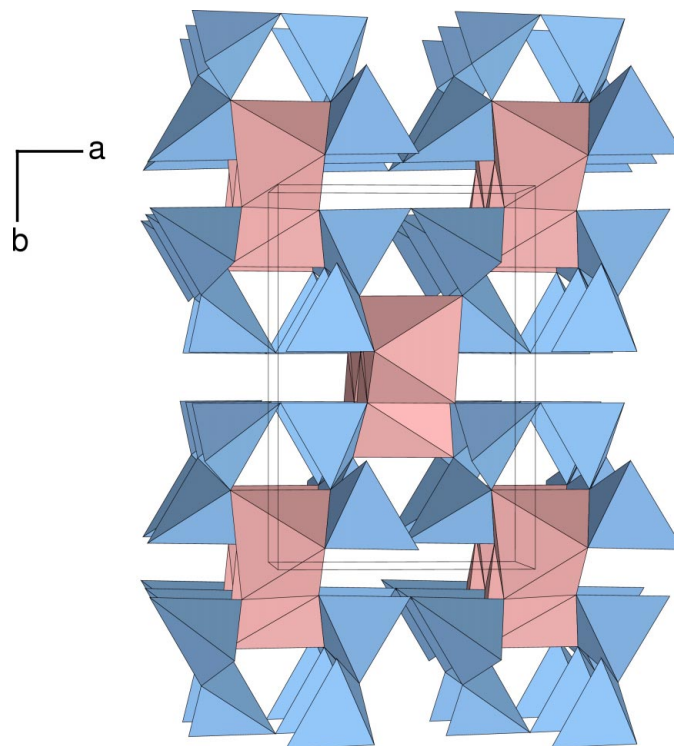
**Figure 2**  
Slice of  $\beta$ - $\text{MnTe}_2\text{O}_5$ , viewed down [010], showing part of an infinite corner-sharing tellurite sheet.

expected value of 2.00. The *trans* O—Mn—O bond angles range from 154.94 (7) to 174.38 (11)°, while the angular variance (Robinson *et al.*, 1971) of the *cis* O—Mn—O angles has the large value of 119.5°.

Te1 (BVS = 4.01, expected 4.00) has three O-atom neighbours with  $d(\text{Te}-\text{O}) < 2.00 \text{ \AA}$  and a further O atom some 2.49 Å distant. This so-called  $\text{TeO}_{3+1}$  coordination approximates to a distorted folded square (or a trigonal bipyramid with one of the equatorial vertices absent and a long axial bond). A similar Te coordination environment has been seen in  $\text{Co}_2\text{Te}_3\text{O}_8$  (Feger *et al.*, 1999). If a fifth, much longer,  $\text{Te1} \cdots \text{O1}^{\text{vii}}$  [ $d = 3.069 (3) \text{ \AA}$ ; symmetry code: (vii)  $-x, 1-y, 1-z$ ] interaction in  $\beta$ - $\text{MnTe}_2\text{O}_5$  is also considered, the Te geometry approximates to a very distorted square-based pyramid. Such asymmetric coordinations are highly characteristic of  $\text{Te}^{\text{IV}}$  and can be correlated with its stereochemically active lone pair of electrons (Brown, 1974).

Of the three O atoms, O1 (site symmetry 2) bridges two Te atoms. O2 bonds to two Te and one Mn in very squashed pyramidal geometry [sum of  $X-\text{O}-X$  ( $X = \text{Mn}, \text{Te}$ ) bond angles = 353.5°] and O3 bonds to two Mn and one Te in essentially planar geometry (sum of  $X-\text{O}-X$  bond angles = 359.4°).

The overall structure of  $\beta$ - $\text{MnTe}_2\text{O}_5$  consists of infinite corrugated sheets of corner-sharing  $\text{TeO}_{3+1}$  moieties propagating in the (010) plane. Connectivity between adjacent



**Figure 3**  
Polyhedral diagram of  $\beta$ - $\text{MnTe}_2\text{O}_5$ , viewed approximately normal to [001]. Colour key:  $\text{MnO}_6$  octahedra pink and  $\text{TeO}_{3+1}$  groups blue.

polyhedra is provided by the O1 and O2 species to result in an anionic layer of stoichiometry  $[\text{Te}_2\text{O}_5]^{2-}$ . These layers contain six-ring (six polyhedral units) loops (Fig. 2). Each  $\text{MnO}_6$  group shares an edge *via* a pair of O3 species [ $d(\text{Mn} \cdots \text{Mn}) = 3.3457 (3) \text{ \AA}$ ] with two others, thus forming infinite chains running in the [001] direction. These Mn octahedral chains serve to fuse the Te layers, *via* edge and corner-sharing, into a three-dimensional network (Fig. 3).

## Experimental

$\text{BaCO}_3$  (0.397 g, 2 mmol),  $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$  (0.793 g, 4 mmol),  $\text{TeO}_2$  (0.957 g, 6 mmol) and 13 ml  $\text{H}_2\text{O}$  were heated to 453 K in a 23-ml capacity, teflon-lined steel bomb for 6 d. The bomb was cooled to room temperature over about 3 h and the resulting solids were recovered by vacuum filtration and rinsing with water. Pink clumps of  $\beta$ - $\text{MnTe}_2\text{O}_5$  crystals were present in the mix, which also included colourless chunks of  $\text{TeO}_2$  and other crystalline phases that are being investigated further. Cuboidal single crystals of  $\beta$ - $\text{MnTe}_2\text{O}_5$  were obtained by gently crushing the clumps between two glass slides.

### Crystal data

$\text{MnTe}_2\text{O}_5$   
 $M_r = 195.07$   
 Orthorhombic,  $Pbcn$   
 $a = 7.3114 (4) \text{ \AA}$   
 $b = 10.9216 (6) \text{ \AA}$   
 $c = 6.1711 (3) \text{ \AA}$   
 $V = 492.78 (5) \text{ \AA}^3$   
 $Z = 4$   
 $D_x = 5.259 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation  
 Cell parameters from 3337 reflections  
 $\theta = 3.3\text{--}32.5^\circ$   
 $\mu = 14.21 \text{ mm}^{-1}$   
 $T = 293 (2) \text{ K}$   
 Cube, pink  
 $0.16 \times 0.15 \times 0.15 \text{ mm}$

## Data collection

Bruker SMART1000 CCD  
diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan  
(*SADABS*; Bruker, 1999)  
 $T_{\min} = 0.210$ ,  $T_{\max} = 0.225$   
3493 measured reflections

890 independent reflections  
863 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.025$   
 $\theta_{\text{max}} = 32.5^\circ$   
 $h = -11 \rightarrow 7$   
 $k = -16 \rightarrow 13$   
 $l = -9 \rightarrow 6$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.019$   
 $wR(F^2) = 0.045$   
 $S = 1.20$   
890 reflections  
39 parameters

$w = 1/[\sigma^2(F_o^2) + (0.021P)^2 + 0.806P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 1.04 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.72 \text{ e } \text{\AA}^{-3}$   
Extinction correction: *SHELXL97*  
Extinction coefficient: 0.0104 (4)

Table 1

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Mn1—O3 <sup>i</sup>	2.154 (2)	Te1—O2	1.8543 (19)
Mn1—O3 <sup>ii</sup>	2.166 (2)	Te1—O1	1.9895 (14)
Mn1—O2	2.2394 (19)	Te1—O2 <sup>iii</sup>	2.490 (2)
Te1—O3	1.8529 (19)		
O3—Te1—O2	98.43 (9)	Te1—O2—Mn1	122.30 (10)
O3—Te1—O1	93.79 (8)	Te1—O2—Te1 <sup>v</sup>	141.25 (10)
O2—Te1—O1	96.24 (9)	Mn1—O2—Te1 <sup>v</sup>	89.90 (6)
O3—Te1—O2 <sup>iii</sup>	77.18 (8)	Te1—O3—Mn1 <sup>vi</sup>	146.49 (11)
O2—Te1—O2 <sup>iii</sup>	98.08 (4)	Te1—O3—Mn1 <sup>iii</sup>	112.46 (10)
O1—Te1—O2 <sup>iii</sup>	164.04 (8)	Mn1 <sup>vi</sup> —O3—Mn1 <sup>iii</sup>	100.48 (8)
Te1 <sup>iv</sup> —O1—Te1	120.37 (14)		

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

The highest difference peak is 0.72  $\text{\AA}$  from Te1 and the deepest difference hole is 1.25  $\text{\AA}$  from Te1.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *ATOMS* (Shape Software, 1999); software used to prepare material for publication: *SHELXL97*.

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