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Key indicators

Single-crystal X-ray study
 $T = 295\text{ K}$
Mean $\sigma(\text{Mg}-\text{O}) = 0.001\text{ \AA}$
 R factor = 0.018
 wR factor = 0.041
Data-to-parameter ratio = 31.0

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

Redetermination of MgTe_2O_5

The crystal structure of the title compound, magnesium pentaoxidotellurate(IV), has been redetermined from a crystal grown from the melt and confirms the previous study [Trömel (1975). *Z. Anorg. Allg. Chem.* **418**, 141–144], but with improved precision. It is isotypic with $\beta\text{-MnTe}_2\text{O}_5$ and contains MgO_6 octahedra and TeO_{3+1} units, with the latter forming an extended sheet structure. Mg and one O atom occupy special positions with site symmetry 2.

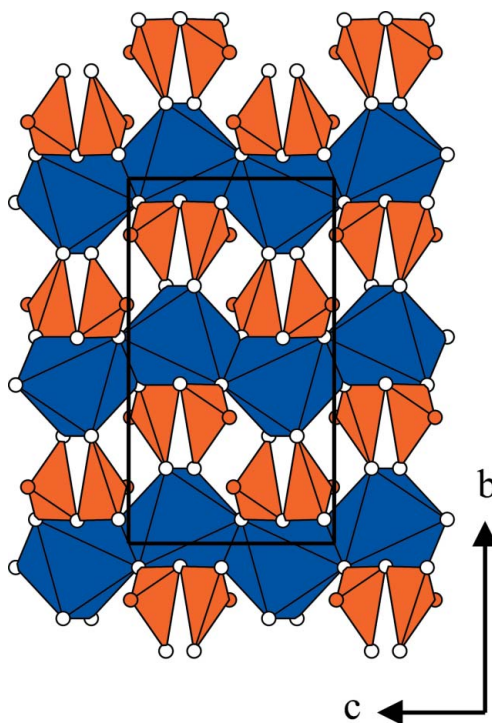
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Comment

The crystal structure of the title compound, (I), has been determined previously by Trömel (1975) by means of intensity data from a two-circle diffractometer. The structure refinement converged with $R(F) = 0.123$ and displacement parameters were not published in the original work. In order to obtain more precise results for comparative studies with other $M\text{Te}_2\text{O}_5$ phases, where M is either an alkaline earth metal (Weil, 2005) or a first-row transition metal [$M = \text{Cu}$ (Hanke *et al.*, 1973), Ni (Platte & Trömel, 1981), Mn (Miletich, 1993; Johnston & Harrison, 2002)], the crystal structure of (I) was

**Figure 1**

The crystal structure of (I) in polyhedral representation, projected along [100]. Note that, for clarity, only short Te–O bonds $< 2.0\text{ \AA}$ were considered for construction of the Te–O polyhedra. Colour key: O atoms white spheres, Te atoms orange spheres, MgO_6 octahedra dark-blue and TeO_3 polyhedra orange.

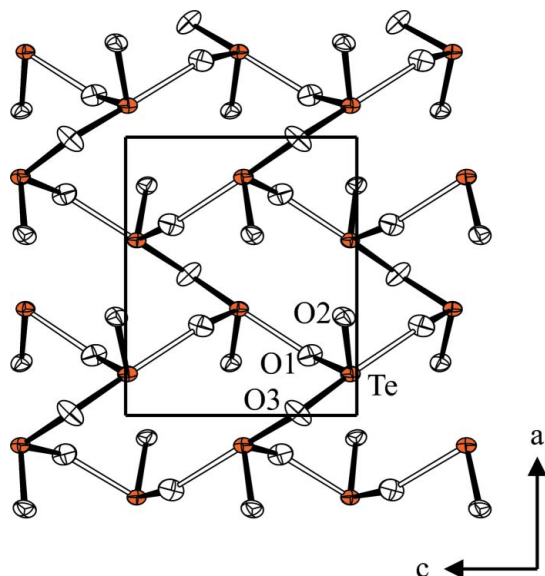


Figure 2

A plot of the two-dimensional Te–O network parallel to the (010) plane. The anisotropic displacement ellipsoids are drawn at the 90% probability level. Short Te–O bonds < 2.0 Å are drawn with closed lines, whereas the longer Te–O bond is drawn with open lines.

reinvestigated. Unlike MnTe_2O_5 , which is known to occur in two modifications, *viz.* denningite-type $\alpha\text{-MnTe}_2\text{O}_5$ (Miletich, 1993) and $\beta\text{-MnTe}_2\text{O}_5$ (Johnston & Harrison, 2002), (I) shows no polymorphism and crystallizes in only one form that is isotypic with $\beta\text{-MnTe}_2\text{O}_5$.

The crystal structure of (I) contains one Mg, one Te and three O atoms in the asymmetric unit, with Mg and one O atom having site symmetry 2. The three-dimensional structure is composed of zigzag chains of edge-sharing MgO_6 octahedra running parallel to the *c* axis, and layers of Te–O polyhedra parallel to the *ac* plane (Fig. 1).

The MgO_6 octahedron in (I) is significantly distorted (Table 1), although the average Mg–O distance of 2.105 Å is in the typical range and in good agreement with the sum of the ionic radii (2.08 Å; Shannon, 1976). The Te atom is coordinated by three O atoms with short Te–O distances < 2 Å (Table 1) and augmented by a fourth O atom at a distance of 2.4048 (13) Å, resulting in a distorted [3 + 1] polyhedron, the geometry of which might be described as a trigonal bipyramid with one equatorial ligand missing and one long axial distance. Similar asymmetric coordination polyhedra are observed for numerous other Te^{IV} oxocompounds and can be correlated with the stereoactive lone pair of electrons. The crystal chemistry of oxotellurate(IV) compounds and the influence of the lone-pair electrons have been discussed in detail in the past (Zemann, 1971; Brown, 1974; Galy *et al.*, 1975; Dolgikh, 1991). The TeO_{3+1} units in (I) share corners to form a two-dimensional anionic network, built from six-membered rings (Fig. 2). The O atoms have coordination numbers of three (O1 and O2) and two (O3). O1 is bonded to two Te and one Mg atom, whereas O2 bridges one Te and two Mg atoms. O3 acts as the bridging atom of two TeO_3 units [$\text{Te}-\text{O}-\text{Te} = 120.91$ (9)°] and is not bonded to Mg.

Results from bond-valence sum (BVS) calculations (Brown, 2002), using the parameters of Brese & O’Keeffe (1991), are in accordance with the expected values: $\text{BVS}(\text{Mg}) = 1.98$ (expected 2.00), $\text{BVS}(\text{Te}_{3+1}) = 4.07$ (4.00), $\text{BVS}(\text{O1}) = 1.99$ (2.00), $\text{BVS}(\text{O2}) = 2.10$ (2.00), $\text{BVS}(\text{O3}) = 1.93$ (2.00).

Experimental

A mixture of MgO (Merck, p.A.) and TeO_2 (Merck, p.A.) in the stoichiometric ratio 1:2 was thoroughly ground and placed in a platinum crucible which was heated in a conventional laboratory furnace for 8 h to 1123 K, kept at that temperature for 2 h and cooled over 96 h to 1023 K. The power was then switched off and the furnace was allowed to cool to room temperature. Colourless chunks of (I), up to 4 mm in length, could be isolated from the light-yellow solidified melt. Spheroidal single crystals were obtained by gentle crushing between two glass slides. Powder X-ray diffraction of the bulk product revealed MgTe_2O_5 as the main phase and TeO_2 in its paratellurite modification as a by-product.

Crystal data

MgTe_2O_5
 $M_r = 359.51$
 Orthorhombic, *Pbcn*
 $a = 7.2391$ (9) Å
 $b = 10.658$ (1) Å
 $c = 5.9880$ (6) Å
 $V = 462.00$ (9) Å³
 $Z = 4$
 $D_x = 5.169$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 25 reflections
 $\theta = 11.3\text{--}16.1^\circ$
 $\mu = 12.68$ mm⁻¹
 $T = 295$ (2) K
 Fragment, colourless
 $0.22 \times 0.22 \times 0.21$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
 $\omega/2\theta$ scans
 Absorption correction: numerical (*HABITUS*; Herrendorf, 1997)
 $T_{\text{min}} = 0.126$, $T_{\text{max}} = 0.242$
 8781 measured reflections
 1210 independent reflections
 1112 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$
 $\theta_{\text{max}} = 37.4^\circ$
 $h = -12 \rightarrow 12$
 $k = -18 \rightarrow 18$
 $l = -10 \rightarrow 10$
 3 standard reflections
 frequency: 300 min
 intensity decay: none

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.018$
 $wR(F^2) = 0.041$
 $S = 1.25$
 1210 reflections
 39 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0172P)^2 + 0.3586P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 1.54$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.62$ e Å⁻³
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.0928 (16)

Table 1

Selected geometric parameters (Å, °).

Mg–O2 ⁱ	2.0801 (13)	Te–O1	1.8588 (12)
Mg–O2 ⁱⁱ	2.0926 (14)	Te–O3	1.9900 (9)
Mg–O1	2.1413 (14)	Te–O1 ⁱⁱⁱ	2.4048 (13)
Te–O2	1.8498 (11)		
O2 ⁱ –Mg–O2 ^{iv}	102.24 (8)	O2–Te–O3	94.00 (5)
O2 ⁱ –Mg–O2 ⁱⁱ	78.62 (5)	O1–Te–O3	96.01 (6)
O2 ^{iv} –Mg–O2 ⁱⁱ	104.82 (5)	O2–Te–O1 ⁱⁱⁱ	76.55 (5)
O2 ⁱⁱ –Mg–O2 ^v	174.67 (8)	O1–Te–O1 ⁱⁱⁱ	98.80 (2)
O2 ⁱ –Mg–O1 ^{vi}	91.08 (5)	O3–Te–O1 ⁱⁱⁱ	163.46 (5)
O2 ^{iv} –Mg–O1 ^{vi}	155.58 (6)	Te–O3–Te ^{vi}	120.91 (9)
O2–Te–O1	98.71 (6)		

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

The atomic coordinates of (I) were taken from the previous refinement (Trömel, 1975) to act as starting parameters. The highest difference peak is 0.51 Å from Te and the deepest hole is 0.63 Å from the same atom. The present study confirms the basic structural features determined from the previous investigation by Trömel (1975) with a much higher precision by about a factor of 10.

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *HELENA* implemented in *PLATON* (Spek, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ATOMS* (Dowty, 2000); software used to prepare material for publication: *SHELXL97*.

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