

The crystal structure of a new CdTe_2O_5 polymorph, isotypic with $\varepsilon\text{-CaTe}_2\text{O}_5$

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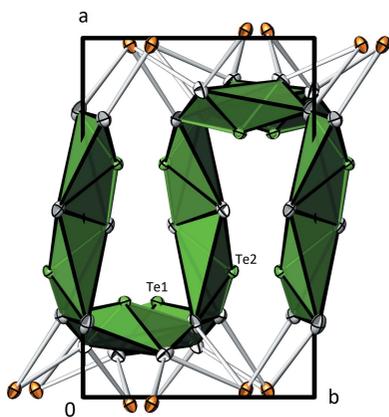
Supporting information: this article has supporting information at journals.iucr.org/e

Single crystals of cadmium pentaoxidoditellurate(IV), CdTe_2O_5 , were obtained as by-products in a hydrothermal reaction of $\text{Cd}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$, TeO_2 , H_6TeO_6 and NH_3 (molar ratios 2:1:1:6) at 483 K for seven days. The crystals represent a different polymorph (henceforth referred to as the β -form) than the α - CdTe_2O_5 crystals grown from the melt, and are isotypic with hydrothermally grown $\varepsilon\text{-CaTe}_2\text{O}_5$. The asymmetric unit of $\beta\text{-CdTe}_2\text{O}_5$ comprises one Cd, two Te and five O sites, all of which are located in general positions (Wyckoff position 4 *e*). The cadmium(II) atom is coordinated by seven oxygen atoms, forming $\infty^2[\text{CdO}_{6/2}\text{O}_{1/1}]$ (100) layers. Both tellurium sites are surrounded by four oxygen atoms with one of them being at a significantly longer distance than the other three. The resulting bisphenoidal $[\text{TeO}_4]$ units also form layers propagating parallel to (100) by sharing edges with each other. The stereochemically active $5s^2$ lone pair of the Te^{IV} atoms leads to the formation of large channels extending along [011] and smaller ones along [010]. A quantitative comparison between the crystal structures of $\beta\text{-CdTe}_2\text{O}_5$ and $\varepsilon\text{-CaTe}_2\text{O}_5$ is made.

1. Chemical context

Cadmium pentaoxidoditellurate(IV), better known under its common name cadmium ditellurite, CdTe_2O_5 , has been the subject of numerous investigations during the past decades with different emphases. In this regard, the $\text{CdO}\text{-TeO}_2$ phase diagram was elucidated by Robertson *et al.* (1978), or the formation of glasses in the $\text{Cd}\text{-Te}\text{-O}$ system by Karaduman *et al.* (2012). Other studies focused on electric and ferroelastic properties of CdTe_2O_5 (Redman *et al.*, 1970), with its ferroelasticity remaining up to the melting point (Sadovskaya *et al.*, 1983; Gorbenko *et al.*, 1990). Single crystals of CdTe_2O_5 are usually grown from the melt utilizing the Czochralski or Bridgeman techniques as crystal growth methods (Nawash, 2015). Even though single crystals of CdTe_2O_5 have been grown for decades this way, a satisfactory structure model for this phase had never been published so far, and only lattice parameters of a sub-cell were given (Redman *et al.*, 1970). Other phases in the $\text{Cd}\text{-Te}\text{-O}$ system that are compiled in the Inorganic Crystal Structure Database (ICSD; Zagorac *et al.*, 2019) include two polymorphs of $\text{CdTe}^{\text{IV}}\text{O}_3$ (Krämer & Brandt, 1985; Poupon *et al.*, 2017), two polymorphs of $\text{Cd}_3\text{Te}^{\text{VI}}\text{O}_6$ (Burckhardt *et al.*, 1982; Weil & Veyer, 2018) and the mixed $\text{Te}^{\text{IV}/\text{VI}}$ -compounds $\text{Cd}_2\text{Te}_2\text{O}_7$ and $\text{Cd}_2\text{Te}_3\text{O}_9$ (Weil, 2004).

The lack of a reasonable structure model for CdTe_2O_5 might be caused by the micaceous appearance of the grown crystals (Redman *et al.*, 1970), as well as by its ferroelastic properties,



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which often are correlated with the formation of twins or multiple domains. The new CdTe₂O₅ phase discovered during the present study originally intended to synthesize new mixed-valent cadmium oxidotellurates(IV,VI), however, belongs to a different polymorph, hereafter referred to as the β-form of CdTe₂O₅.

In this communication we report on the synthesis and crystal structure analysis of β-CdTe₂O₅ and compare it quantitatively with the isotypic structure of ε-CaTe₂O₅ (Weil & Stöger, 2008; Barrier *et al.*, 2009).

2. Structural commentary

All atoms in the asymmetric unit, *viz.* one Cd site, two Te sites and five O sites, are located on general Wyckoff positions 4 *e* (site symmetry 1). The cadmium atom is coordinated by seven oxygen atoms with distances in a range of 2.235 (3)–2.688 (3) Å. The average Cd–O bond length is 2.389 Å, which is in accordance with the sum of ionic radii for Cd^{II} (CN 7; 1.17 Å) and O (CN 3; 1.22 Å) compiled by Shannon (1976). The bond-valence sum (BVS; Brown, 2002) of Cd is 2.07 valence units (v.u.) using the values of Brese & O’Keeffe (1991) for calculation. The [CdO₇] polyhedron is best described as a distorted pentagonal bipyramid (Fig. 1). The [CdO₇] polyhedra are connected to each other by sharing three edges with other [CdO₇] units, thereby forming ∞²[CdO_{6/2}O_{1/1}] layers oriented parallel to (100) with the Cd^{II} atoms located at *x* ≈ 0;1.

The two tellurium(IV) atoms are both coordinated by four oxygen atoms with three of them being closer than 2 Å (Table 1) and the fourth one at a distance of 2.285 (3) Å (Te1) and 2.204 (3) Å (Te2), respectively. The oxygen atoms are located to one side of the Te^{IV} atoms due to the large amount

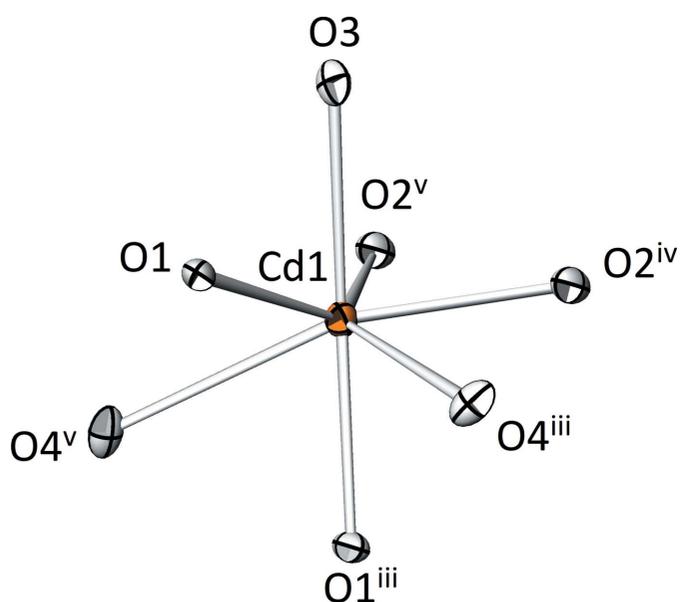


Figure 1
The [CdO₇] polyhedron in the crystal structure of β-CdTe₂O₅. Displacement ellipsoids are drawn at the 90% probability level. Symmetry codes refer to Table 1.

Table 1
Comparison of Te–O and *M*–O (*M* = Cd, Ca) bond lengths (Å) in the isotypic β-CdTe₂O₅ and ε-CaTe₂O₅ structures.

| | β-CdTe ₂ O ₅ | ε-CaTe ₂ O ₅ ^a |
|----------------------|------------------------------------|---|
| Te1–O2 | 1.843 (3) | 1.832 (4) |
| Te1–O1 | 1.875 (3) | 1.852 (4) |
| Te1–O3 | 1.991 (3) | 1.980 (5) |
| Te1–O4 | 2.285 (3) | 2.450 (5) |
| Te2–O4 ⁱ | 1.864 (3) | 1.854 (4) |
| Te2–O5 | 1.897 (3) | 1.898 (4) |
| Te2–O3 | 1.990 (3) | 2.009 (5) |
| Te2–O5 ⁱⁱ | 2.204 (5) | 2.178 (5) |
| M1–O1 ⁱⁱⁱ | 2.235 (3) | 2.305 (4) |
| M1–O2 ^{iv} | 2.238 (3) | 2.326 (4) |
| M1–O1 | 2.256 (3) | 2.360 (5) |
| M1–O2 ^v | 2.296 (3) | 2.358 (5) |
| M1–O3 | 2.424 (3) | 2.476 (5) |
| M1–O4 ^v | 2.589 (3) | 2.554 (5) |
| M1–O4 ⁱⁱⁱ | 2.688 (3) | 2.682 (5) |

(*a*) Lattice parameters: *a* = 9.382 (2), *b* = 5.7095 (14), *c* = 11.132 (3) Å, β = 115.109 (4)°, *V* = 539.95 Å³ (Weil & Stöger, 2008). [Symmetry codes: (i) *x*, $-y + \frac{1}{2}$, $z - \frac{1}{2}$; (ii) $-x + 1$, $-y + 1$, $-z + 1$; (iii) $-x$, $y + \frac{1}{2}$, $-z + 1$; (iv) $-x$, $-y + 1$, $-z + 1$; (v) *x*, *y* + 1, *z*.]

of space the 5s² electron lone pair requires. The corresponding coordination polyhedra can be derived from a trigonal bipyramid, [ΨTeO₄], with the lone pair occupying one of the equatorial positions in each case. The shapes of the polyhedra without the contribution of the lone pair correspond to [TeO₄] bisphenoids (Fig. 2). The bond-valence sums for the tellurium(IV) atoms were calculated to be 4.15 and 4.10 v.u. for Te1 and Te2, respectively, using the values of Brese & O’Keeffe (1991). When applying the revised parameters of Mills & Christy (2013), BVS of 3.94 and 3.92 v.u. were obtained.

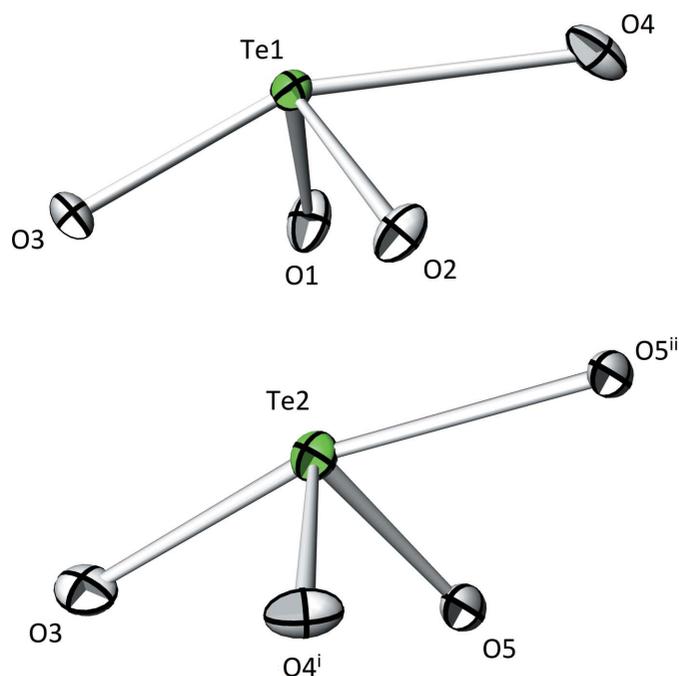


Figure 2
The [TeO₄] polyhedra in the crystal structure of β-CdTe₂O₅. Displacement ellipsoids are drawn at the 90% probability level. Symmetry codes refer to Table 1.

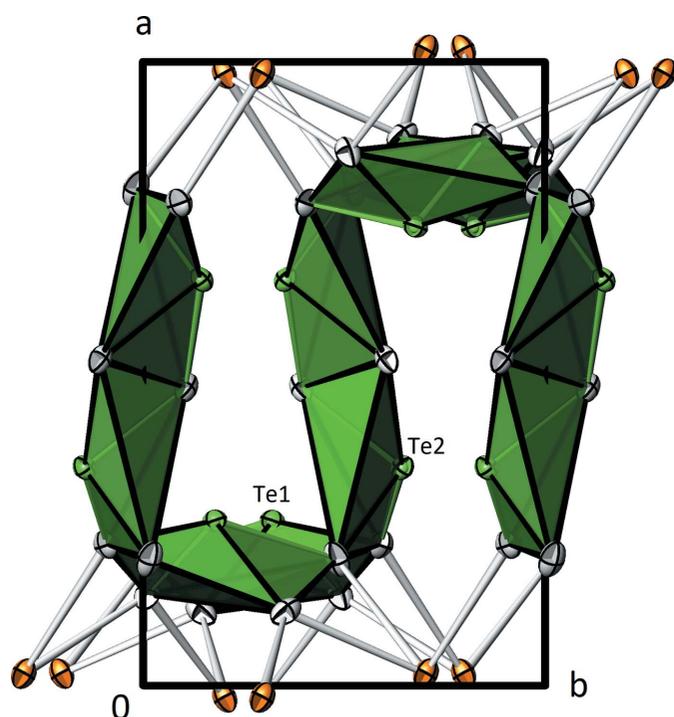


Figure 3
The crystal structure of β - CdTe_2O_5 in a projection along [001]. Displacement ellipsoids are drawn at the 90% probability level.

The $[\text{TeO}_4]$ polyhedra are connected to each other to form layers oriented parallel to (100). These layers have a distinct undulating shape (Fig. 3) and are built up by chains of $[\text{Te1O}_4]$ and $[\text{Te2O}_4]$ units arranged alternately by sharing corners with two neighbours. These chains are cross-linked by two $[\text{Te2O}_4]$ -polyhedra by sharing an edge consisting of two O5 atoms. The $[\text{Te1O}_4]$ units are located very close to the Cd–O layer and share edges with three $[\text{CdO}_7]$ polyhedra and one corner with a fourth one. The $[\text{Te2O}_4]$ units are positioned in the centre of the layer and only share two corners with three $[\text{CdO}_7]$ polyhedra. The rather loose arrangement of $[\text{TeO}_4]$ units in the layer can be explained by the stereochemically active $5s^2$

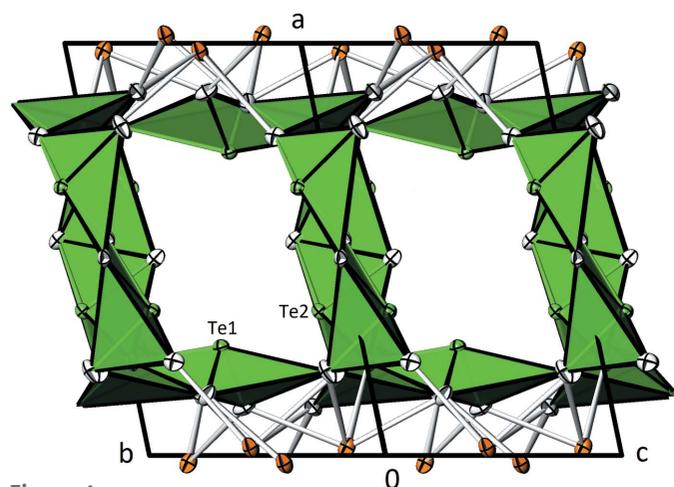


Figure 4
Large channels in the β - CdTe_2O_5 structure running parallel to [011]. Displacement ellipsoids are drawn at the 90% probability level.

electron lone pair situated at each of the two Te^{IV} atoms. The space requirements of the non-bonding electron pairs lead to the undulating shape of the layer, which results in the presence of large channels in the structure, which are oriented parallel to [011] (Fig. 4). Smaller channels are also realized and propagate parallel to [010] (Fig. 5).

The arrangement of such an undulating ${}^2_{\infty}[\text{Te}_2\text{O}_5]^{2-}$ layer was reported for the first time for the ε -polymorph of CaTe_2O_5 (Weil & Stöger, 2008), which is isotopic with β - CdTe_2O_5 . CaTe_2O_5 is likewise reported to crystallize in a mica-like form from the melt (Redman *et al.*, 1970). Although several high-temperature polymorphs have also been reported for this phase (Tripathi *et al.*, 2001), ε - CaTe_2O_5 is the only polymorph for which a crystal-structure determination has been performed (Weil & Stöger, 2008; Barrier *et al.*, 2009). The close similarity between the two structures can be explained by the very similar ionic radii (Shannon, 1976) of Ca (CN 7: 1.20 Å) and Cd (CN 7: 1.17 Å). The corresponding bond lengths in the isotopic structures (Table 1) differ only slightly with one exception: the Te1–O4 bond, which is 0.165 Å longer in the Ca structure, shows by far the biggest difference. A quantitative comparison between β - CdTe_2O_5 and ε - CaTe_2O_5 was carried out using the *compstru* software (de la Flor *et al.*, 2016), available at the Bilbao Crystallographic Server (Aroyo *et al.*, 2006). The absolute distances between paired atoms are 0.0303 Å for Cd/Ca1, 0.0628 Å for Te1, 0.0178 Å for Te2, 0.1426 Å for O1, 0.0791 Å for O2, 0.0384 Å for O3, 0.0788 Å for O4 and 0.0635 Å for O5. The degree of lattice distortion is 0.0118, the arithmetic mean of the distance between paired atoms is 0.0642 Å, and the measure of similarity is 0.077.

3. Synthesis and crystallization

Crystals of CdTe_2O_5 were obtained under hydrothermal conditions. The reactants, 0.1890 g (0.613 mmol)

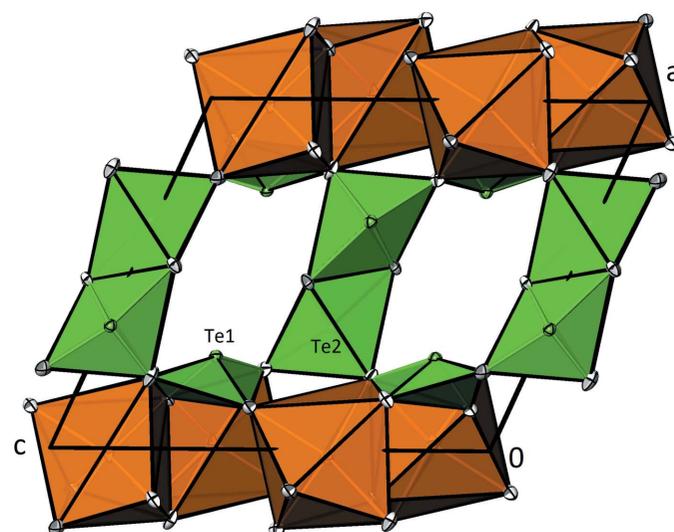


Figure 5
Smaller channels in the β - CdTe_2O_5 structure running parallel to [010]. Displacement ellipsoids are drawn at the 90% probability level.

Table 2
Experimental details.

| | |
|--|---|
| Crystal data | |
| Chemical formula | CdTe ₂ O ₅ |
| <i>M_r</i> | 447.60 |
| Crystal system, space group | Monoclinic, <i>P2₁/c</i> |
| Temperature (K) | 100 |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 9.4535 (5), 5.5806 (3), 10.8607 (5) |
| β (°) | 114.430 (1) |
| <i>V</i> (Å ³) | 521.67 (5) |
| <i>Z</i> | 4 |
| Radiation type | Mo <i>K</i> α |
| μ (mm ⁻¹) | 15.08 |
| Crystal size (mm) | 0.10 × 0.06 × 0.05 |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015) |
| <i>T_{min}</i> , <i>T_{max}</i> | 0.600, 0.746 |
| No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections | 9236, 1827, 1462 |
| <i>R_{int}</i> | 0.045 |
| (sin θ/λ) _{max} (Å ⁻¹) | 0.747 |
| Refinement | |
| <i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i> | 0.024, 0.045, 1.00 |
| No. of reflections | 1827 |
| No. of parameters | 73 |
| $\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³) | 1.20, -1.04 |

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b), *ATOMS* (Dowty, 2006), *publCIF* (Westrip, 2010).

Cd(NO₃)₂·2H₂O, 0.0484 g (0.303 mmol) TeO₂, 0.0710 g (0.309 mmol) H₆TeO₆ and 0.12 g (1.8 mmol) 25%_{wt} NH_{3(aq)} were weighed into a small teflon vessel with a volume of ca 3 ml. Deionized water was added until the vessel was filled to about two thirds of its volume. Then the vessel was heated to 483 K in a steel autoclave for 7 d under autogenous pressure. Afterwards, the autoclave was cooled to room temperature within about 4 h. The reaction product was a light-yellow, almost white solid. In the X-ray powder pattern of the bulk, α-Cd₃TeO₆ (Burckhardt *et al.*, 1982) and β-CdTe₂O₅ were found. Under a polarising microscope a few small shiny colourless blocks of β-CdTe₂O₅ were isolated for single-crystal measurements.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Atom labels and starting coord-

inates for refinement were adopted from the isotypic ε-CaTe₂O₅ structure (Weil & Stöger, 2008).

Acknowledgements

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supporting information

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The crystal structure of a new CdTe₂O₅ polymorph, isotypic with ϵ -CaTe₂O₅

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINTE* (Bruker, 2016); data reduction: *SAINTE* (Bruker, 2016); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *ATOMS* (Dowty, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Cadmium pentaoxidoditellurate(IV)

Crystal data

| | |
|----------------------------------|---|
| CdTe ₂ O ₅ | $F(000) = 768$ |
| $M_r = 447.60$ | $D_x = 5.699 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| $a = 9.4535 (5) \text{ \AA}$ | Cell parameters from 2645 reflections |
| $b = 5.5806 (3) \text{ \AA}$ | $\theta = 2.4\text{--}32.1^\circ$ |
| $c = 10.8607 (5) \text{ \AA}$ | $\mu = 15.08 \text{ mm}^{-1}$ |
| $\beta = 114.430 (1)^\circ$ | $T = 100 \text{ K}$ |
| $V = 521.67 (5) \text{ \AA}^3$ | Block, colourless |
| $Z = 4$ | $0.10 \times 0.06 \times 0.05 \text{ mm}$ |

Data collection

| | |
|--|--|
| Bruker APEXII CCD diffractometer | 1827 independent reflections |
| ω - and φ -scan | 1462 reflections with $I > 2\sigma(I)$ |
| Absorption correction: multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015) | $R_{\text{int}} = 0.045$ |
| $T_{\text{min}} = 0.600$, $T_{\text{max}} = 0.746$ | $\theta_{\text{max}} = 32.1^\circ$, $\theta_{\text{min}} = 3.8^\circ$ |
| 9236 measured reflections | $h = -14 \rightarrow 14$ |
| | $k = -8 \rightarrow 8$ |
| | $l = -15 \rightarrow 16$ |

Refinement

| | |
|---------------------------------|---|
| Refinement on F^2 | Primary atom site location: isomorphous structure methods |
| Least-squares matrix: full | $w = 1/[\sigma^2(F_o^2) + (0.0171P)^2]$ |
| $R[F^2 > 2\sigma(F^2)] = 0.024$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.045$ | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| $S = 1.00$ | $\Delta\rho_{\text{max}} = 1.20 \text{ e \AA}^{-3}$ |
| 1827 reflections | $\Delta\rho_{\text{min}} = -1.03 \text{ e \AA}^{-3}$ |
| 73 parameters | |
| 0 restraints | |

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|-------------|-------------|----------------------------------|
| Te1 | 0.25911 (3) | 0.32034 (5) | 0.72297 (3) | 0.01195 (7) |
| Te2 | 0.34935 (3) | 0.64780 (5) | 0.49078 (3) | 0.01181 (7) |
| Cd1 | 0.01900 (4) | 0.79762 (6) | 0.63620 (3) | 0.01416 (8) |
| O1 | 0.1293 (4) | 0.4948 (5) | 0.7821 (3) | 0.0141 (6) |
| O2 | 0.1216 (4) | 0.1359 (5) | 0.5843 (3) | 0.0188 (7) |
| O3 | 0.2239 (4) | 0.5960 (5) | 0.5973 (3) | 0.0163 (7) |
| O4 | 0.2081 (4) | 0.0287 (6) | 0.8466 (3) | 0.0162 (7) |
| O5 | 0.4791 (4) | 0.3979 (6) | 0.5962 (3) | 0.0176 (7) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|---------------|--------------|---------------|
| Te1 | 0.00997 (13) | 0.01304 (14) | 0.01191 (13) | 0.00123 (10) | 0.00360 (10) | −0.00069 (10) |
| Te2 | 0.01214 (13) | 0.01187 (13) | 0.01070 (13) | −0.00178 (10) | 0.00399 (10) | −0.00077 (10) |
| Cd1 | 0.01824 (16) | 0.01311 (16) | 0.01254 (15) | 0.00370 (12) | 0.00778 (13) | 0.00255 (12) |
| O1 | 0.0171 (16) | 0.0124 (15) | 0.0175 (15) | 0.0035 (12) | 0.0116 (13) | 0.0054 (12) |
| O2 | 0.0256 (18) | 0.0146 (16) | 0.0109 (15) | −0.0055 (14) | 0.0023 (13) | −0.0008 (13) |
| O3 | 0.0199 (17) | 0.0142 (15) | 0.0209 (16) | 0.0035 (13) | 0.0144 (14) | 0.0032 (13) |
| O4 | 0.0162 (16) | 0.0142 (15) | 0.0159 (15) | 0.0016 (13) | 0.0044 (13) | 0.0068 (13) |
| O5 | 0.0162 (16) | 0.0198 (16) | 0.0188 (16) | 0.0060 (13) | 0.0094 (13) | 0.0072 (13) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|-------------------------|-------------|--|-------------|
| Te1—O2 | 1.843 (3) | Te2—Te2 ⁱⁱ | 3.2253 (6) |
| Te1—O1 | 1.875 (3) | Cd1—O1 ⁱⁱⁱ | 2.235 (3) |
| Te1—O3 | 1.991 (3) | Cd1—O2 ^{iv} | 2.238 (3) |
| Te1—O4 | 2.285 (3) | Cd1—O2 ^v | 2.296 (3) |
| Te2—O4 ⁱ | 1.864 (3) | Cd1—O1 | 2.255 (3) |
| Te2—O5 | 1.897 (3) | Cd1—O3 | 2.424 (3) |
| Te2—O3 | 1.990 (3) | Cd1—O4 ^v | 2.589 (3) |
| Te2—O5 ⁱⁱ | 2.204 (3) | Cd1—O4 ⁱⁱⁱ | 2.688 (3) |
| O2—Te1—O1 | 103.25 (15) | O1 ⁱⁱⁱ —Cd1—O3 | 167.39 (11) |
| O2—Te1—O3 | 90.59 (13) | O2 ^{iv} —Cd1—O3 | 93.09 (12) |
| O1—Te1—O3 | 83.46 (12) | O2 ^v —Cd1—O3 | 83.66 (11) |
| O2—Te1—O4 | 80.40 (12) | O1—Cd1—O3 | 66.67 (10) |
| O1—Te1—O4 | 80.89 (12) | O1 ⁱⁱⁱ —Cd1—O4 ^v | 73.85 (11) |
| O3—Te1—O4 | 159.60 (12) | O2 ^{iv} —Cd1—O4 ^v | 138.57 (10) |
| O4 ⁱ —Te2—O5 | 100.25 (14) | O2 ^v —Cd1—O4 ^v | 66.40 (10) |

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| O4 ⁱ —Te2—O3 | 91.11 (13) | O1—Cd1—O4 ^v | 78.65 (10) |
| O5—Te2—O3 | 86.24 (13) | O3—Cd1—O4 ^v | 94.31 (10) |
| O4 ⁱ —Te2—O5 ⁱⁱ | 88.71 (13) | Te1—O1—Cd1 ^{vi} | 119.15 (14) |
| O5—Te2—O5 ⁱⁱ | 76.52 (13) | Te1—O1—Cd1 | 109.06 (13) |
| O3—Te2—O5 ⁱⁱ | 162.43 (12) | Cd1 ^{vi} —O1—Cd1 | 117.64 (13) |
| O4 ⁱ —Te2—Te2 ⁱⁱ | 95.12 (10) | Te1—O2—Cd1 ^{iv} | 133.44 (16) |
| O5—Te2—Te2 ⁱⁱ | 41.63 (9) | Te1—O2—Cd1 ^{vii} | 119.05 (14) |
| O3—Te2—Te2 ⁱⁱ | 127.79 (9) | Cd1 ^{iv} —O2—Cd1 ^{vii} | 105.95 (12) |
| O5 ⁱⁱ —Te2—Te2 ⁱⁱ | 34.89 (8) | Te1—O3—Te2 | 122.67 (15) |
| O1 ⁱⁱⁱ —Cd1—O2 ^{iv} | 98.69 (12) | Te1—O3—Cd1 | 99.09 (12) |
| O1 ⁱⁱⁱ —Cd1—O2 ^v | 95.20 (12) | Te2—O3—Cd1 | 138.18 (14) |
| O2 ^{iv} —Cd1—O2 ^v | 74.05 (13) | Te2 ^{viii} —O4—Te1 | 128.18 (16) |
| O1 ⁱⁱⁱ —Cd1—O1 | 105.89 (7) | Te2 ^{viii} —O4—Cd1 ^{vii} | 118.13 (14) |
| O2 ^{iv} —Cd1—O1 | 140.67 (11) | Te1—O4—Cd1 ^{vii} | 94.15 (10) |
| O2 ^v —Cd1—O1 | 131.97 (12) | Te2—O5—Te2 ⁱⁱ | 103.48 (13) |

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