

Received 2 October 2018

Accepted 8 October 2018

Edited by A. Van der Lee, Université de
Montpellier II, France**Keywords:** crystal structure; dimorphism;
 Mg_3TeO_6 structure type; solid solution.**CCDC reference:** 1872058**Supporting information:** this article has
supporting information at journals.iucr.org/e

A new form of Cd_3TeO_6 revealing dimorphism

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Phase-formation studies in the system $\text{CdO}\text{--}\text{TeO}_3$ using a CsCl/NaCl melt at comparatively low temperatures revealed that tricadmium orthotellurate(VI), Cd_3TeO_6 , is dimorphic. The new modification of Cd_3TeO_6 is denoted as the β -form and adopts the rhombohedral Mg_3TeO_6 structure type with one Cd and two O sites in general positions, and two Te sites with site symmetry $\bar{3}$ each. In comparison with the previously reported monoclinic cryolite-type α -form that was prepared at higher temperatures, $\beta\text{-Cd}_3\text{TeO}_6$ has a much lower density and most likely represents a metastable modification. Whereas the $[\text{TeO}_6]$ octahedra in both polymorphs are very similar and show only minor deviations from ideal values, the polyhedra around the Cd^{II} sites are different, with a distorted $[\text{CdO}_6]$ octahedron in both modifications but an additional $[\text{CdO}_8]$ polyhedron with a $[4 + 4]$ coordination in the α -form.

1. Chemical context

Various salts of *meta*-telluric acid, H_2TeO_4 , have been reported as a result of high-pressure and high-temperature experiments (3000 atm; 973 K) aiming at various $M^{\text{II}}\text{TeO}_4$ phases, where $M = \text{Mg}, \text{Ca}, \text{Sr}, \text{Ba}, \text{Cd}$ or Pb (Sleight *et al.*, 1972). Meanwhile, the crystal structures of the Ca, Sr and Ba salts were determined (Hottentot & Loopstra, 1979; Weil *et al.*, 2016) whereas those of the other phases remain unknown to date. In a recent project on single-crystal growth of the Cd salt of *meta*-telluric acid, we used a CsCl/NaCl salt mixture (Żemczużny & Rambach, 1909) at temperatures < 800 K as a flux. Instead of the target phase CdTeO_4 , we obtained a new form of Cd_3TeO_6 . The previously reported Cd_3TeO_6 polymorph crystallizes as a monoclinically distorted cryolite-type material in space-group type $P2_1/n$ (Burckhardt *et al.*, 1982) while the new form adopts the rhombohedral Mg_3TeO_6 structure type.

Prior to the current study, solid solutions $\text{Cd}_{3-x}\text{Mn}_x\text{TeO}_6$ with $x = 3, 2, 1.5$ and 1 were prepared in polycrystalline form (Ivanov *et al.*, 2012), but not the cadmium end member, *i.e.* where $x = 0$. We report here the crystal structure of the new polymorph of Cd_3TeO_6 , together with a comparative discussion of isostructural solid solutions $\text{Cd}_{3-x}\text{Mn}_x\text{TeO}_6$. In the following, we refer to the previously reported monoclinic polymorph of Cd_3TeO_6 (Burckhardt *et al.*, 1982) as the α -form, and the new rhombohedral polymorph as the β -form of Cd_3TeO_6 .

2. Structural commentary

The crystal structure of $\beta\text{-Cd}_3\text{TeO}_6$ (Fig. 1) is made up from a distorted close packing of hexagonal oxygen layers extending

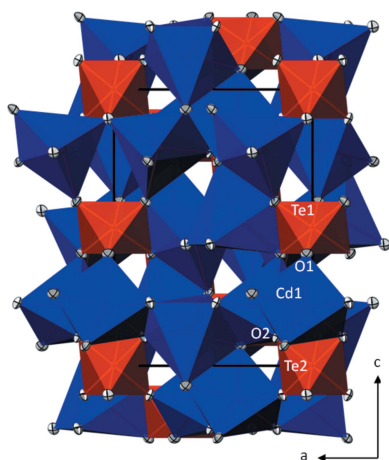


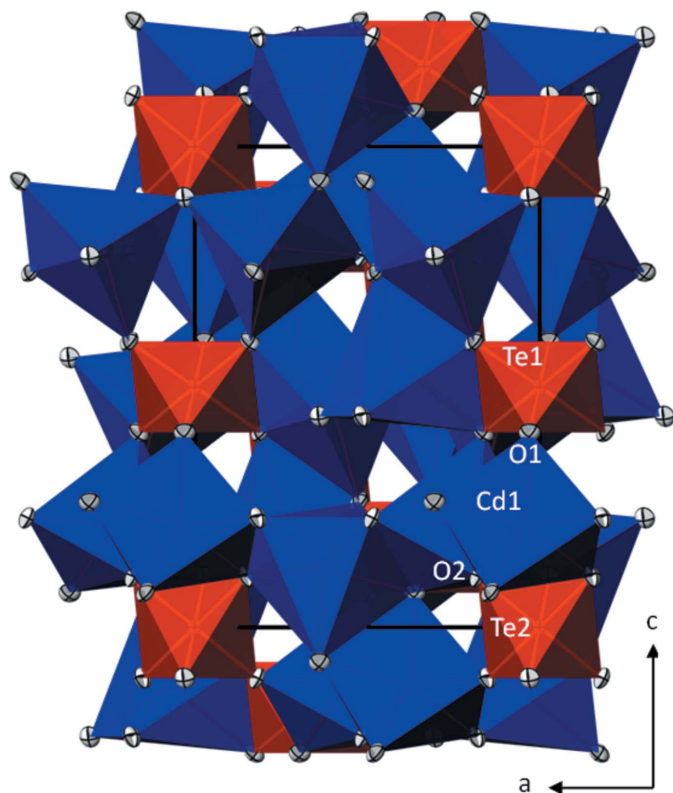
Table 1

 Selected bond lengths (Å) in rhombohedral β -Cd₃TeO₆ and in isotypic (Cd_{1.5}Mn_{1.5})TeO₆ and Mn₃TeO₆.

	β -Cd ₃ TeO ₆ ^a	Cd _{1.5} Mn _{1.5} TeO ₆ ^b	Mn ₃ TeO ₆ ^c
M1—O1	2.2348 (17)	2.147	2.1055 (14)
M1—O2 ⁱ	2.2455 (17)	2.150	2.1275 (13)
M1—O1 ⁱⁱ	2.2907 (19)	2.240	2.2009 (13)
M1—O2 ⁱⁱⁱ	2.3051 (18)	2.260	2.2311 (12)
M1—O2	2.3370 (18)	2.273	2.2313 (13)
M1—O1 ^{iv}	2.4658 (19)	2.412	2.3841 (13)
Te1—O1	1.9339 (17)	1.955	1.9247 (13)
Te2—O2	1.9290 (17)	1.959	1.9214 (12)

Notes: (a) This study; (b) Ivanov *et al.* (2012) on the basis of X-ray powder diffraction data at room temperature (no s.u. given in original publication); (c) Weil (2006) on the basis of single-crystal X-ray data at room temperature. [Symmetry codes: (i) $y - \frac{1}{3}, -x + y + \frac{1}{3}, -z + \frac{2}{3}$; (ii) $-x + \frac{2}{3}, y + \frac{2}{3}, -z + \frac{2}{3}$; (iii) $-y, x - y, z$; (iv) $-y + \frac{1}{3}, x - y + \frac{2}{3}, z - \frac{1}{3}$]

parallel to (001). The Cd site (site symmetry 1) and the two unique Te sites (each with site symmetry $\bar{3}$) are situated in the octahedral interstices of this arrangement. The distorted [CdO₆] octahedron has Cd—O distances ranging from 2.2348 (17)–2.4658 (19) Å (Table 1) and shares one edge with a [Te1O₆] octahedron, another edge with a [Te2O₆] octahedron, and four edges with neighbouring [CdO₆] octahedra. Both [TeO₆] octahedra show only minute deviations from the ideal octahedral symmetry. They are isolated from each other and are connected to six [CdO₆] octahedra by sharing edges. The average Te—O bond length in β -Cd₃TeO₆ (1.931 Å) is in


Figure 1

The crystal structure of β -Cd₃TeO₆ in polyhedral view in a projection along [010]. [CdO₆] octahedra are blue and [TeO₆] octahedra are red. Displacement ellipsoids are drawn at the 90% probability level.

very good agreement with the mean Te—O bond length of 1.923 Å calculated for numerous (> 100) oxotellurates with octahedrally coordinated Te^{VI} (Christy *et al.*, 2016; Gagné & Hawthorne, 2018). Both unique O atoms are bonded to one Te and three Cd atoms in the form of a distorted tetrahedron.

Like β -Cd₃TeO₆, Mn₃TeO₆ (Weil, 2006) as well as phases with $x = 2, 1.5$ and 1 of the Cd_{3-x}Mn_xTeO₆ solid-solution series (Ivanov *et al.*, 2012) adopt the rhombohedral Mg₃TeO₆ structure type. A comparison of the bond lengths of the [MO₆] ($M = \text{Cd, Mn}$) octahedra in the end members β -Cd₃TeO₆ and Mn₃TeO₆ and the solid solution Cd_{1.5}Mn_{1.5}TeO₆ (mixed occupancy for the M site) shows intermediate values for the solid solution, consistent with the different ionic radii for six-coordinate Cd^{II} and Mn^{II} of 0.95 and 0.83 (high-spin) Å, respectively (Shannon, 1976). For a quantitative structural comparison of the end members β -Cd₃TeO₆ and Mn₃TeO₆ the program *compstru* (de la Flor *et al.*, 2016) available at the Bilbao Crystallographic Server (Aroyo *et al.*, 2006) was used. The degree of lattice distortion is 0.0204, the maximum distance between the atomic positions of paired atoms is 0.0680 Å for pair O2, the arithmetic mean of all distances is 0.0417 Å, and the measure of similarity is 0.011. All these values show a high similarity between the two crystal structures.

The structure of the monoclinic α -form of Cd₃TeO₆ (Burckhardt *et al.*, 1982) comprises of two cadmium sites (one on a general position and one on an inversion centre), one tellurium site on an inversion centre and three oxygen sites in general positions. While the [TeO₆] octahedra in both Cd₃TeO₆ polymorphs have nearly the same bond length distribution [2×1.904 (4), 2×1.924 (5), 2×1.948 (4) Å in the α -form; for the β -form, see: Table 1], the set of coordination polyhedra around the two Cd^{II} cations in the two structures is different. In β -Cd₃TeO₆, the cadmium site has a coordination number (CN) of six with an octahedral oxygen environment whereas in α -Cd₃TeO₆, only one site is octahedrally surrounded [range of Cd—O bond lengths: 2.211 (5)–2.350 (4) Å] and the other site exhibits a distorted [4 + 4] coordination [range of Cd—O bond lengths: 2.237 (5)–3.010 (5) Å].

As noted above, the end members β -Cd₃TeO₆ and Mn₃TeO₆ crystallize in the same structure type, suggesting a full miscibility over the complete range of x for the solid-solution series Cd_{3-x}Mn_xTeO₆. However, the adopted structure type for the complete range of x appears to be dependent on the reaction temperature. Single crystals of α -Cd₃TeO₆ for structure analysis were grown from a 9 CdO: 11 TeO₂ mixture that was heated in air at 1350 K for three h (Burckhardt *et al.*, 1982) while single crystals of β -Cd₃TeO₆ were obtained at much lower temperatures (793 K) using a flux method. This suggests that the high-temperature synthesis yields the thermodynamically stable modification. The rule of thumb that in the majority of cases the denser polymorph represents also the thermodynamically stable modification supports this assumption because α -Cd₃TeO₆ [$D_x = 7.490$ (2) g cm⁻³; Burckhardt *et al.*, 1982] is much denser than β -Cd₃TeO₆ [$D_x = 6.941$ g cm⁻³]. Under consideration of the similar reaction conditions for

Table 2
Experimental details.

Crystal data	
Chemical formula	Cd ₃ TeO ₆
<i>M_r</i>	560.80
Crystal system, space group	Trigonal, <i>R</i> $\bar{3}$: <i>H</i>
Temperature (K)	296
<i>a</i> , <i>c</i> (Å)	9.1620 (2), 11.0736 (3)
<i>V</i> (Å ³)	805.01 (4)
<i>Z</i>	6
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	17.06
Crystal size (mm)	0.08 (radius)
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> _{min} , <i>T</i> _{max}	0.527, 0.749
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	11351, 1623, 1526
<i>R</i> _{int}	0.033
(sin θ/λ) _{max} (Å ⁻¹)	1.025
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.023, 0.046, 1.29
No. of reflections	1623
No. of parameters	33
Δρ _{max} , Δρ _{min} (e Å ⁻³)	2.57, -1.53

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXL2017/1* (Sheldrick, 2015), *ATOMS for Windows* (Dowty, 2006) and *pubCIF* (Westrip, 2010).

preparation of monoclinic α-Cd₃TeO₆ and the given solid solutions Cd_{3-x}Mn_xTeO₆ (1270 K following a ceramic route; Ivanov *et al.*, 2012), it appears likely that the rhombohedral β-Cd₃TeO₆ end member can be prepared only at lower temperatures whereas certain amounts of manganese substituting cadmium in the Cd_{3-x}Mn_xTeO₆ solid-solution series stabilize the Mg₃TeO₆ structure type at higher temperatures. Unfortunately, because of the scarcity of β-Cd₃TeO₆ material, a detailed investigation of the thermal behaviour of this phase, *e.g.* in terms of stability and a possible phase transition to α-Cd₃TeO₆, could not be undertaken.

3. Database survey

According to a search of the Inorganic Crystal Structure Database (ICSD; Belsky *et al.*, 2002), the Mg₃TeO₆ structure type is realized for eponymous Mg₃TeO₆ (Schulz & Bayer, 1971), Ca₃UO₆ (Holc & Golic, 1983), Mn₃WO₆ (Klüver & Müller-Buschbaum, 1994), Li₃AlD₆ (Brinks & Hauback, 2003; Løvvik *et al.*, 2004), Mn₃TeO₆ (Weil, 2006), selected solid solutions Cd_{3-x}Mn_xTeO₆ (Ivanov *et al.*, 2012), Mn_{3-x}Co_xTeO₆ (Singh *et al.*, 2014; Ivanov *et al.*, 2014), Mn_{2.4}Cu_{0.6}TeO₆ (Wulff *et al.*, 1998), (Ca_{0.2667}Y_{0.7333})₃(Y_{0.2}Sn_{0.3})Sn_{0.5}O₆ (Kaminaga *et al.*, 2006), Mn₂InSbO₆ and Mn₂ScSbO₆ (Ivanov *et al.*, 2011), Sc₃(Sc_{0.295}Al_{0.705})O₆ (Müller *et al.*, 2004) and Ho₃ScO₆ (Badie, 1973).

4. Synthesis and crystallization

The rhombohedral β-form of Cd₃TeO₆ was obtained as one of the products from a flux synthesis using a CsCl/NaCl salt

mixture (molar ratio 0.65/0.35). To 1.7 g of the salt mixture were added CdO (0.13 g) and TeO₃ (0.18 g). TeO₃ had previously been prepared by heating H₆TeO₆ at 573 K for 8 h. The reaction mixture was evacuated and sealed in a silica ampoule, heated from room temperature within 3 h to 793 K, kept at that temperature for 90 h and cooled within 10 h back to room temperature. The silica ampoule was subsequently broken and the solidified melt leached out with water for 2 h. The off-white product was filtered off, washed with water and was air-dried. The title compound was present in the form of a few nearly spherical colourless crystals. Other phases identified by single-crystal X-ray diffraction measurements of selected crystals were α-Cd₃TeO₆ (Burckhardt *et al.*, 1982), the mixed-valent Te^{IV/VI} compound Cd₂Te₂O₇ (Weil, 2004) and a new form of incommensurately modulated CdTe₂O₅ (Weil & Stöger, 2018). Estimated on optical inspection with a microscope, all these phases represent minor by-products. Powder X-ray diffraction measurements of the bulk additionally revealed triple-perovskite-type CsCdCl₃ (Siegel & Gebert, 1964) as the main phase and the Te^{IV} compound CdTeO₃ (Krämer & Brandt, 1985) as a minority phase. Some additional reflections in the X-ray powder diffraction pattern of the bulk could not be assigned to the phases mentioned above or to any other known phase(s).

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Standardized coordinates (Gelato & Parthé, 1987) from the isotypic phase Mn₃TeO₆ (Weil, 2006) were taken as starting parameters for refinement. The highest and lowest remaining electron density peaks are located 1.56 and 1.53 Å from sites Te2 and O1, respectively.

Acknowledgements

The X-ray centre of the TU Wien is acknowledged for financial support and for providing access to the single-crystal and powder X-ray diffractometers.

Funding information

TV acknowledges the Erasmus+ programme for an educational exchange.

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supporting information

Acta Cryst. (2018). E74, 1561-1564 [https://doi.org/10.1107/S2056989018014214]

A new form of Cd₃TeO₆ revealing dimorphism

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Computing details

Data collection: *APEX3* (Bruker, 2015); cell refinement: *SAINT* (Bruker, 2015); data reduction: *SAINT* (Bruker, 2015); program(s) used to solve structure: coordinates from isotypic structure; program(s) used to refine structure: *SHELXL2017/1* (Sheldrick, 2015); molecular graphics: *ATOMS for Windows* (Dowty, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Tricadmium orthotellurate(VI)

Crystal data

Cd ₃ TeO ₆	$D_x = 6.941 \text{ Mg m}^{-3}$
$M_r = 560.80$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Trigonal, $R\bar{3}:H$	Cell parameters from 6637 reflections
$a = 9.1620 (2) \text{ \AA}$	$\theta = 5.0\text{--}46.6^\circ$
$c = 11.0736 (3) \text{ \AA}$	$\mu = 17.06 \text{ mm}^{-1}$
$V = 805.01 (4) \text{ \AA}^3$	$T = 296 \text{ K}$
$Z = 6$	Spherical, colourless
$F(000) = 1464$	$0.08 \times 0.08 \times 0.08 \times 0.08$ (radius) mm

Data collection

Bruker APEXII CCD diffractometer	1623 independent reflections
ω - and φ -scans	1526 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)	$R_{\text{int}} = 0.033$
$T_{\text{min}} = 0.527$, $T_{\text{max}} = 0.749$	$\theta_{\text{max}} = 46.8^\circ$, $\theta_{\text{min}} = 3.2^\circ$
11351 measured reflections	$h = -18 \rightarrow 18$
	$k = -18 \rightarrow 16$
	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0021P)^2 + 11.2674P]$
Least-squares matrix: full	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.023$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$wR(F^2) = 0.046$	$\Delta\rho_{\text{max}} = 2.57 \text{ e \AA}^{-3}$
$S = 1.29$	$\Delta\rho_{\text{min}} = -1.53 \text{ e \AA}^{-3}$
1623 reflections	Extinction correction: <i>SHELXL-2017/1</i>
33 parameters	(Sheldrick 2015),
0 restraints	$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.00434 (9)

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>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.03947 (2)	0.26424 (2)	0.21210 (2)	0.00731 (4)
Te1	0.000000	0.000000	0.500000	0.00444 (5)
Te2	0.000000	0.000000	0.000000	0.00424 (5)
O1	0.0289 (2)	0.1903 (2)	0.40560 (16)	0.0087 (2)
O2	0.1800 (2)	0.1509 (2)	0.10570 (16)	0.0078 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.00657 (6)	0.00745 (6)	0.00789 (6)	0.00348 (5)	-0.00052 (4)	-0.00099 (4)
Te1	0.00419 (7)	0.00419 (7)	0.00492 (10)	0.00210 (3)	0.000	0.000
Te2	0.00403 (7)	0.00403 (7)	0.00464 (10)	0.00202 (3)	0.000	0.000
O1	0.0102 (6)	0.0074 (6)	0.0082 (5)	0.0043 (5)	-0.0001 (5)	0.0024 (4)
O2	0.0058 (5)	0.0069 (6)	0.0094 (6)	0.0021 (5)	-0.0024 (4)	-0.0017 (4)

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

Cd1—O1	2.2348 (17)	Te1—O1 ^{viii}	1.9339 (18)
Cd1—O2 ⁱ	2.2455 (17)	Te1—O1 ⁱⁱⁱ	1.9339 (17)
Cd1—O1 ⁱⁱ	2.2907 (19)	Te1—O1 ^{ix}	1.9339 (17)
Cd1—O2 ⁱⁱⁱ	2.3051 (18)	Te1—O1 ^x	1.9339 (17)
Cd1—O2	2.3370 (18)	Te1—O1 ^{xi}	1.9339 (17)
Cd1—O1 ^{iv}	2.4658 (19)	Te1—O1	1.9339 (17)
Cd1—Te2	3.2608 (2)	Te2—O2	1.9290 (17)
Cd1—Te1 ^v	3.3420 (2)	Te2—O2 ^{xii}	1.9290 (17)
Cd1—Cd1 ⁱⁱ	3.3606 (3)	Te2—O2 ⁱⁱⁱ	1.9290 (17)
Cd1—Cd1 ^{vi}	3.4239 (3)	Te2—O2 ^{xiii}	1.9291 (17)
Cd1—Cd1 ^{vii}	3.4537 (2)	Te2—O2 ^{xiv}	1.9291 (17)
Cd1—Cd1 ⁱ	3.4538 (2)	Te2—O2 ^{xi}	1.9291 (17)
O1—Cd1—O2 ⁱ	94.05 (7)	O1 ^x —Te1—Cd1 ^{xvii}	79.65 (6)
O1—Cd1—O1 ⁱⁱ	84.10 (7)	O1 ^{xi} —Te1—Cd1 ^{xvii}	100.35 (6)
O2 ⁱ —Cd1—O1 ⁱⁱ	120.35 (7)	O1—Te1—Cd1 ^{xvii}	138.37 (6)
O1—Cd1—O2 ⁱⁱⁱ	107.98 (7)	Cd1 ^{xv} —Te1—Cd1 ^{xvii}	117.776 (1)
O2 ⁱ —Cd1—O2 ⁱⁱⁱ	82.41 (7)	Cd1 ^{xvi} —Te1—Cd1 ^{xvii}	62.224 (1)
O1 ⁱⁱ —Cd1—O2 ⁱⁱⁱ	154.11 (6)	Cd1 ⁱⁱ —Te1—Cd1 ^{xvii}	180.0
O1—Cd1—O2	107.37 (6)	O1 ^{viii} —Te1—Cd1 ^{xviii}	100.35 (6)
O2 ⁱ —Cd1—O2	148.88 (4)	O1 ⁱⁱⁱ —Te1—Cd1 ^{xviii}	79.65 (6)
O1 ⁱⁱ —Cd1—O2	84.88 (6)	O1 ^{ix} —Te1—Cd1 ^{xviii}	46.92 (5)

O2 ⁱⁱⁱ —Cd1—O2	69.79 (8)	O1 ^x —Te1—Cd1 ^{xviii}	138.37 (6)
O1—Cd1—O1 ^{iv}	144.36 (6)	O1 ^{xi} —Te1—Cd1 ^{xviii}	41.63 (6)
O2 ⁱ —Cd1—O1 ^{iv}	82.90 (6)	O1—Te1—Cd1 ^{xviii}	133.08 (5)
O1 ⁱⁱ —Cd1—O1 ^{iv}	67.58 (8)	Cd1 ^{xv} —Te1—Cd1 ^{xviii}	62.225 (1)
O2 ⁱⁱⁱ —Cd1—O1 ^{iv}	106.78 (6)	Cd1 ^{xvi} —Te1—Cd1 ^{xviii}	117.775 (1)
O2—Cd1—O1 ^{iv}	91.75 (6)	Cd1 ⁱⁱ —Te1—Cd1 ^{xviii}	117.775 (1)
O1—Cd1—Te2	119.57 (5)	Cd1 ^{xvii} —Te1—Cd1 ^{xviii}	62.225 (1)
O2 ⁱ —Cd1—Te2	113.76 (5)	O1 ^{viii} —Te1—Cd1 ^{xix}	79.65 (6)
O1 ⁱⁱ —Cd1—Te2	118.53 (5)	O1 ⁱⁱⁱ —Te1—Cd1 ^{xix}	100.35 (6)
O2 ⁱⁱⁱ —Cd1—Te2	35.59 (4)	O1 ^{ix} —Te1—Cd1 ^{xix}	133.08 (5)
O2—Cd1—Te2	35.72 (4)	O1 ^x —Te1—Cd1 ^{xix}	41.63 (6)
O1 ^{iv} —Cd1—Te2	93.60 (4)	O1 ^{xi} —Te1—Cd1 ^{xix}	138.37 (6)
O1—Cd1—Te1 ^v	111.58 (5)	O1—Te1—Cd1 ^{xix}	46.92 (5)
O2 ⁱ —Cd1—Te1 ^v	97.31 (5)	Cd1 ^{xv} —Te1—Cd1 ^{xix}	117.775 (1)
O1 ⁱⁱ —Cd1—Te1 ^v	34.11 (4)	Cd1 ^{xvi} —Te1—Cd1 ^{xix}	62.225 (1)
O2 ⁱⁱⁱ —Cd1—Te1 ^v	140.34 (4)	Cd1 ⁱⁱ —Te1—Cd1 ^{xix}	62.225 (1)
O2—Cd1—Te1 ^v	95.47 (4)	Cd1 ^{xvii} —Te1—Cd1 ^{xix}	117.775 (1)
O1 ^{iv} —Cd1—Te1 ^v	34.95 (4)	Cd1 ^{xviii} —Te1—Cd1 ^{xix}	180.0
Te2—Cd1—Te1 ^v	116.088 (5)	O2—Te2—O2 ^{xii}	93.00 (8)
O1—Cd1—Cd1 ⁱⁱ	42.69 (5)	O2—Te2—O2 ⁱⁱⁱ	87.00 (8)
O2 ⁱ —Cd1—Cd1 ⁱⁱ	113.04 (5)	O2 ^{xii} —Te2—O2 ⁱⁱⁱ	180.00 (11)
O1 ⁱⁱ —Cd1—Cd1 ⁱⁱ	41.41 (4)	O2—Te2—O2 ^{xiii}	180.0
O2 ⁱⁱⁱ —Cd1—Cd1 ⁱⁱ	144.94 (5)	O2 ^{xii} —Te2—O2 ^{xiii}	87.00 (8)
O2—Cd1—Cd1 ⁱⁱ	97.92 (4)	O2 ⁱⁱⁱ —Te2—O2 ^{xiii}	93.00 (8)
O1 ^{iv} —Cd1—Cd1 ⁱⁱ	106.29 (4)	O2—Te2—O2 ^{xiv}	93.00 (8)
Te2—Cd1—Cd1 ⁱⁱ	130.823 (8)	O2 ^{xii} —Te2—O2 ^{xiv}	87.00 (8)
Te1 ^v —Cd1—Cd1 ⁱⁱ	71.352 (5)	O2 ⁱⁱⁱ —Te2—O2 ^{xiv}	93.00 (8)
O1—Cd1—Cd1 ^{vi}	104.72 (5)	O2 ^{xiii} —Te2—O2 ^{xiv}	87.00 (8)
O2 ⁱ —Cd1—Cd1 ^{vi}	41.86 (5)	O2—Te2—O2 ^{xi}	87.00 (8)
O1 ⁱⁱ —Cd1—Cd1 ^{vi}	159.57 (5)	O2 ^{xii} —Te2—O2 ^{xi}	93.00 (8)
O2 ⁱⁱⁱ —Cd1—Cd1 ^{vi}	40.55 (4)	O2 ⁱⁱⁱ —Te2—O2 ^{xi}	87.00 (8)
O2—Cd1—Cd1 ^{vi}	109.20 (4)	O2 ^{xiii} —Te2—O2 ^{xi}	93.00 (8)
O1 ^{iv} —Cd1—Cd1 ^{vi}	96.51 (4)	O2 ^{xiv} —Te2—O2 ^{xi}	180.00 (13)
Te2—Cd1—Cd1 ^{vi}	73.547 (5)	O2—Te2—Cd1 ^{xiii}	134.98 (5)
Te1 ^v —Cd1—Cd1 ^{vi}	126.995 (8)	O2 ^{xii} —Te2—Cd1 ^{xiii}	44.06 (5)
Cd1 ⁱⁱ —Cd1—Cd1 ^{vi}	143.877 (10)	O2 ⁱⁱⁱ —Te2—Cd1 ^{xiii}	135.94 (5)
O1—Cd1—Cd1 ^{vii}	104.17 (5)	O2 ^{xiii} —Te2—Cd1 ^{xiii}	45.02 (5)
O2 ⁱ —Cd1—Cd1 ^{vii}	153.98 (5)	O2 ^{xiv} —Te2—Cd1 ^{xiii}	96.56 (5)
O1 ⁱⁱ —Cd1—Cd1 ^{vii}	45.47 (5)	O2 ^{xi} —Te2—Cd1 ^{xiii}	83.44 (5)
O2 ⁱⁱⁱ —Cd1—Cd1 ^{vii}	108.67 (4)	O2—Te2—Cd1 ^{xi}	44.06 (5)
O2—Cd1—Cd1 ^{vii}	40.10 (4)	O2 ^{xii} —Te2—Cd1 ^{xi}	83.44 (5)
O1 ^{iv} —Cd1—Cd1 ^{vii}	71.44 (4)	O2 ⁱⁱⁱ —Te2—Cd1 ^{xi}	96.56 (5)
Te2—Cd1—Cd1 ^{vii}	73.148 (6)	O2 ^{xiii} —Te2—Cd1 ^{xi}	135.94 (5)
Te1 ^v —Cd1—Cd1 ^{vii}	58.887 (1)	O2 ^{xiv} —Te2—Cd1 ^{xi}	134.98 (5)
Cd1 ⁱⁱ —Cd1—Cd1 ^{vii}	71.628 (5)	O2 ^{xi} —Te2—Cd1 ^{xi}	45.02 (5)
Cd1 ^{vi} —Cd1—Cd1 ^{vii}	143.600 (10)	Cd1 ^{xiii} —Te2—Cd1 ^{xi}	106.152 (5)
O1—Cd1—Cd1 ⁱ	122.01 (5)	O2—Te2—Cd1	45.02 (5)
O2 ⁱ —Cd1—Cd1 ⁱ	42.10 (5)	O2 ^{xii} —Te2—Cd1	135.94 (5)

O1 ⁱⁱ —Cd1—Cd1 ⁱ	90.20 (4)	O2 ⁱⁱⁱ —Te2—Cd1	44.06 (5)
O2 ⁱⁱⁱ —Cd1—Cd1 ⁱ	101.62 (5)	O2 ^{xiii} —Te2—Cd1	134.98 (5)
O2—Cd1—Cd1 ⁱ	129.56 (4)	O2 ^{xiv} —Te2—Cd1	83.44 (5)
O1 ^{iv} —Cd1—Cd1 ⁱ	41.48 (4)	O2 ^{xi} —Te2—Cd1	96.56 (5)
Te2—Cd1—Cd1 ⁱ	113.622 (7)	Cd1 ^{xiii} —Te2—Cd1	180.0
Te1 ^v —Cd1—Cd1 ⁱ	58.888 (1)	Cd1 ^{xi} —Te2—Cd1	73.847 (5)
Cd1 ⁱⁱ —Cd1—Cd1 ⁱ	110.788 (6)	O2—Te2—Cd1 ^{xiv}	135.94 (5)
Cd1 ^{vi} —Cd1—Cd1 ⁱ	69.450 (8)	O2 ^{xii} —Te2—Cd1 ^{xiv}	96.56 (5)
Cd1 ^{vii} —Cd1—Cd1 ⁱ	111.882 (5)	O2 ⁱⁱⁱ —Te2—Cd1 ^{xiv}	83.44 (5)
O1 ^{viii} —Te1—O1 ⁱⁱⁱ	180.0	O2 ^{xiii} —Te2—Cd1 ^{xiv}	44.06 (5)
O1 ^{viii} —Te1—O1 ^{ix}	93.54 (7)	O2 ^{xiv} —Te2—Cd1 ^{xiv}	45.02 (5)
O1 ⁱⁱⁱ —Te1—O1 ^{ix}	86.46 (7)	O2 ^{xi} —Te2—Cd1 ^{xiv}	134.98 (5)
O1 ^{viii} —Te1—O1 ^x	93.54 (7)	Cd1 ^{xiii} —Te2—Cd1 ^{xiv}	73.848 (5)
O1 ⁱⁱⁱ —Te1—O1 ^x	86.46 (7)	Cd1 ^{xi} —Te2—Cd1 ^{xiv}	180.0
O1 ^{ix} —Te1—O1 ^x	93.54 (7)	Cd1—Te2—Cd1 ^{xiv}	106.153 (5)
O1 ^{viii} —Te1—O1 ^{xi}	86.46 (7)	O2—Te2—Cd1 ^{xii}	83.44 (5)
O1 ⁱⁱⁱ —Te1—O1 ^{xi}	93.54 (7)	O2 ^{xii} —Te2—Cd1 ^{xii}	45.02 (5)
O1 ^{ix} —Te1—O1 ^{xi}	86.46 (7)	O2 ⁱⁱⁱ —Te2—Cd1 ^{xii}	134.98 (5)
O1 ^x —Te1—O1 ^{xi}	180.0	O2 ^{xiii} —Te2—Cd1 ^{xii}	96.56 (5)
O1 ^{viii} —Te1—O1	86.46 (7)	O2 ^{xiv} —Te2—Cd1 ^{xii}	44.06 (5)
O1 ⁱⁱⁱ —Te1—O1	93.54 (7)	O2 ^{xi} —Te2—Cd1 ^{xii}	135.94 (5)
O1 ^{ix} —Te1—O1	180.0	Cd1 ^{xiii} —Te2—Cd1 ^{xii}	73.848 (5)
O1 ^x —Te1—O1	86.46 (7)	Cd1 ^{xi} —Te2—Cd1 ^{xii}	106.152 (5)
O1 ^{xi} —Te1—O1	93.54 (7)	Cd1—Te2—Cd1 ^{xii}	106.153 (5)
O1 ^{viii} —Te1—Cd1 ^{xv}	41.63 (6)	Cd1 ^{xiv} —Te2—Cd1 ^{xii}	73.848 (5)
O1 ⁱⁱⁱ —Te1—Cd1 ^{xv}	138.37 (6)	O2—Te2—Cd1 ⁱⁱⁱ	96.56 (5)
O1 ^{ix} —Te1—Cd1 ^{xv}	79.65 (6)	O2 ^{xii} —Te2—Cd1 ⁱⁱⁱ	134.98 (5)
O1 ^x —Te1—Cd1 ^{xv}	133.08 (6)	O2 ⁱⁱⁱ —Te2—Cd1 ⁱⁱⁱ	45.02 (5)
O1 ^{xi} —Te1—Cd1 ^{xv}	46.92 (6)	O2 ^{xiii} —Te2—Cd1 ⁱⁱⁱ	83.44 (5)
O1—Te1—Cd1 ^{xv}	100.35 (6)	O2 ^{xiv} —Te2—Cd1 ⁱⁱⁱ	135.94 (5)
O1 ^{viii} —Te1—Cd1 ^{xvi}	138.37 (6)	O2 ^{xi} —Te2—Cd1 ⁱⁱⁱ	44.06 (5)
O1 ⁱⁱⁱ —Te1—Cd1 ^{xvi}	41.63 (6)	Cd1 ^{xiii} —Te2—Cd1 ⁱⁱⁱ	106.152 (5)
O1 ^{ix} —Te1—Cd1 ^{xvi}	100.35 (6)	Cd1 ^{xi} —Te2—Cd1 ⁱⁱⁱ	73.848 (5)
O1 ^x —Te1—Cd1 ^{xvi}	46.92 (6)	Cd1—Te2—Cd1 ⁱⁱⁱ	73.847 (5)
O1 ^{xi} —Te1—Cd1 ^{xvi}	133.08 (6)	Cd1 ^{xiv} —Te2—Cd1 ⁱⁱⁱ	106.152 (5)
O1—Te1—Cd1 ^{xvi}	79.65 (6)	Cd1 ^{xii} —Te2—Cd1 ⁱⁱⁱ	180.000 (11)
Cd1 ^{xv} —Te1—Cd1 ^{xvi}	180.0	Te1—O1—Cd1	139.23 (10)
O1 ^{viii} —Te1—Cd1 ⁱⁱ	46.92 (5)	Te1—O1—Cd1 ⁱⁱ	104.25 (8)
O1 ⁱⁱⁱ —Te1—Cd1 ⁱⁱ	133.08 (5)	Cd1—O1—Cd1 ⁱⁱ	95.90 (7)
O1 ^{ix} —Te1—Cd1 ⁱⁱ	138.37 (6)	Te1—O1—Cd1 ^{xix}	98.13 (7)
O1 ^x —Te1—Cd1 ⁱⁱ	100.35 (6)	Cd1—O1—Cd1 ^{xix}	116.00 (7)
O1 ^{xi} —Te1—Cd1 ⁱⁱ	79.65 (6)	Cd1 ⁱⁱ —O1—Cd1 ^{xix}	93.05 (7)
O1—Te1—Cd1 ⁱⁱ	41.63 (6)	Te2—O2—Cd1 ^{vii}	147.03 (10)
Cd1 ^{xv} —Te1—Cd1 ⁱⁱ	62.223 (1)	Te2—O2—Cd1 ^{xi}	100.35 (7)
Cd1 ^{xvi} —Te1—Cd1 ⁱⁱ	117.776 (1)	Cd1 ^{vii} —O2—Cd1 ^{xi}	97.59 (7)
O1 ^{viii} —Te1—Cd1 ^{xvii}	133.08 (5)	Te2—O2—Cd1	99.25 (7)

$O1^{iii}-Te1-Cd1^{xvii}$	46.92 (5)	$Cd1^{vii}-O2-Cd1$	97.80 (7)
$O1^{ix}-Te1-Cd1^{xvii}$	41.63 (6)	$Cd1^{xi}-O2-Cd1$	115.12 (8)

Symmetry codes: (i) $y-1/3, -x+y+1/3, -z+1/3$; (ii) $-x+1/3, -y+2/3, -z+2/3$; (iii) $-y, x-y, z$; (iv) $-y+1/3, x-y+2/3, z-1/3$; (v) $x+1/3, y+2/3, z-1/3$; (vi) $-x-1/3, -y+1/3, -z+1/3$; (vii) $x-y+2/3, x+1/3, -z+1/3$; (viii) $y, -x+y, -z+1$; (ix) $-x, -y, -z+1$; (x) $x-y, x, -z+1$; (xi) $-x+y, -x, z$; (xii) $y, -x+y, -z$; (xiii) $-x, -y, -z$; (xiv) $x-y, x, -z$; (xv) $-y+2/3, x-y+1/3, z+1/3$; (xvi) $y-2/3, -x+y-1/3, -z+2/3$; (xvii) $x-1/3, y-2/3, z+1/3$; (xviii) $x-y+1/3, x-1/3, -z+2/3$; (xix) $-x+y-1/3, -x+1/3, z+1/3$.