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$Ca_2Te_3O_8$, a new phase in the CaO–TeO_2 system

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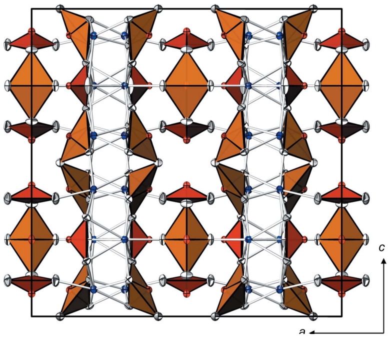
Single crystals of dicalcium octaoxidotritellurate(IV), $Ca_2Te_3O_8$, were obtained from a CsCl/NaCl melt with CaO and TeO_2 as educts in the molar ratio of 1:2. $Ca_2Te_3O_8$ crystallizes isotypically with $Pb_3Te_2O_8$ and is comprised of two unique Ca, four Te and eight O sites. One calcium cation has eight and the other nine coordination partners. Both coordination polyhedra are considerably distorted. Two kinds of oxotellurate(IV) anions with the same formula $[Te_3O_8]^{4-}$ are present. One is an infinite zigzag chain anion consisting of pairs of $[TeO_4]$ bisphenoids linked to a trigonal–pyramidal $[TeO_3]$ group with a connectivity of $[(TeO_{1/1}O_{2/2})(TeO_{2/1}O_{2/2})_2]_n$, while the other is a finite anion made up of one central $[TeO_4]$ bisphenoid linked to two $[TeO_3]$ trigonal pyramids and has a connectivity of $[(TeO_{2/1}O_{1/2})_2(TeO_{2/2}O_{2/1})]$. In the crystal, the anions are organized in layers extending parallel to (100). Adjacent layers are held together by the calcium cations to define a three-dimensional framework structure.



1. Chemical context

A partial phase diagram for the pseudo-binary system CaO–TeO_2 has been determined for the composition range 50–100 mol% TeO_2 to contain the 1:1 phase $CaTeO_3$ and the 1:2 phase $CaTe_2O_5$ (Mishra *et al.*, 1998). Another phase not reported during the original study of Mishra *et al.* (1998) is the 4:5 phase $Ca_4Te_5O_{14}$, for which full structural details were determined for the normal-pressure and high-pressure forms (Weil, 2004; Weil *et al.*, 2016). For compositions $CaTeO_3$ and $CaTe_2O_5$, polymorphism was reported on the basis of differential thermal analysis and temperature-dependent X-ray diffracion (Mishra *et al.*, 1998; Tripathi *et al.*, 2001), however, without structural details of the corresponding phases. Whereas crystal structure determinations were subsequently performed for four polymorphic forms of $CaTeO_3$ (Stöger *et al.*, 2009; Poupon *et al.*, 2015), our present knowledge of the $CaTe_2O_5$ structures is restricted to only one form (Weil & Stöger, 2008; Barrier *et al.*, 2009) that is not related to the mica-like $CaTe_2O_5$ phase reported nearly 50 years ago (Redman *et al.*, 1970). In an attempt to grow single crystals of the latter from a salt melt at comparatively low temperatures, a heretofore unknown phase in the CaO–TeO_2 system was obtained, *viz.* the 2:3 phase $Ca_2Te_3O_8$.

In this article, preparation conditions, crystal structure and the relation to the isotypic lead(II) analogue $Pb_2Te_3O_8$ (Champarnaud-Mesjard *et al.*, 2001) are reported.

2. Structural commentary

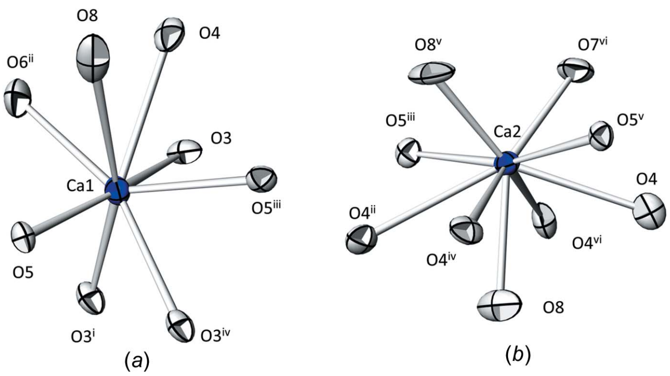
The asymmetric unit of $Ca_2Te_3O_8$ comprises two Ca sites, four Te sites and eight O sites. One Ca site (Ca2) is located on Wyckoff position 8*g* (site symmetry ..*m*), sites Te1 on 4*c*

Table 1
Comparison of bond lengths (Å) in $Ca_2Te_3O_8$ and isotypic $Pb_2Te_3O_8$.

	$\mathbf{Ca_2Te_3O_8}$[a]	$\mathbf{Pb_2Te_3O_8}$[b]
$M1—O3^{\text{i}}$	2.3198 (11)	2.372 (8)
$M1—O6^{\text{ii}}$	2.3903 (13)	2.440 (8)
$M1—O5$	2.3924 (11)	2.470 (6)
$M1—O3$	2.4691 (12)	2.636 (8)
$M1—O5^{\text{iii}}$	2.4712 (11)	2.934 (8)
$M1—O3^{\text{iv}}$	2.6212 (12)	3.032 (8)
$M1—O4$	2.7186 (13)	
$M1—O8$	3.0360 (4)	3.069 (2)
$M2—O8^{\text{v}}$	2.3089 (18)	2.439 (9)
$M2—O7^{\text{vi}}$	2.3660 (17)	2.374 (10)
$M2—O5^{\text{v}}$	2.4497 (11)	2.556 (6)
$M2—O5^{\text{iii}}$	2.4497 (11)	2.556 (6)
$M2—O8$	2.4749 (19)	3.080 (11)
$M2—O4^{\text{vi}}$	2.6335 (13)	2.732 (6)
$M2—O4^{\text{iv}}$	2.6335 (13)	2.732 (6)
$M2—O4$	2.9154 (13)	3.342 (7)
$M2—O4^{\text{ii}}$	2.9154 (13)	3.342 (7)
$Te1—O7^{\text{vii}}$	1.8369 (17)	1.852 (10)
$Te1—O7^{\text{viii}}$	1.8369 (17)	1.852 (10)
$Te1—O1$	2.1608 (17)	2.160 (9)
$Te1—O1^{\text{ii}}$	2.1608 (17)	2.160 (9)
$Te2—O6^{\text{ix}}$	1.8522 (12)	1.859 (8)
$Te2—O6$	1.8522 (12)	1.859 (8)
$Te2—O1$	1.8902 (17)	1.883 (10)
$Te3—O3$	1.8602 (11)	1.868 (8)
$Te3—O5^{x}$	1.8743 (10)	1.856 (7)
$Te3—O2^{x}$	2.0123 (5)	2.008 (3)
$Te3—O4$	2.3222 (12)	2.338 (6)
$Te4—O8$	1.8694 (17)	1.857 (10)
$Te4—O4$	1.8994 (11)	1.900 (7)
$Te4—O4^{\text{ii}}$	1.8994 (11)	1.900 (7)

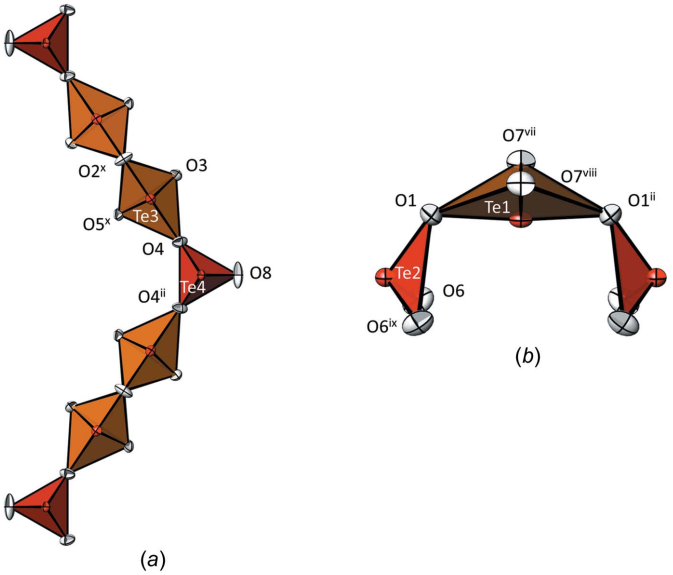
Notes: (*a*) this study; (*b*) Champarnaud-Mesjard *et al.* (2001); single-crystal data with a = 19.522 (4), b = 7.121 (1) and c = 18.813 (4) Å. Symmetry codes: (i) $x, -y+1, -z+1$; (ii) $x, y, -z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, z$; (iv) $-x+\frac{1}{2}, y-\frac{1}{2}, z$; (v) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (vi) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (vii) $x, y-1, z$; (viii) $-x+1, y-1, -z+\frac{1}{2}$; (ix) $-x+1, y, z$; (*x*) $x, y+1, z$.

(*m*2*m*), Te2 on 8*f* (*m*..), Te4 on 8*g*, O1 on 8*f*, O2 on 8*e* (2..) and O7 and O8 both on 8*g*; all other sites are on general positions 16*h*.



(*a*) (*b*)

Figure 1
(*a*) The $[Ca1O_8]$ and (*b*) the $[Ca1O_9]$ polyhedra in the crystal structure of $Ca_2Te_3O_8$. Displacement ellipsoids are drawn at the 90% probability level. Symmetry codes refer to Table 1.



(*a*) (*b*)

Figure 2
(*a*) The chain $[Te_3O_8]^{4-}$ anion and (*b*) the finite $[Te_3O_8]^{4-}$ anion in the crystal structure of $Ca_2Te_3O_8$. Displacement ellipsoids are drawn at the 90% probability level. Symmetry codes refer to Table 1.

The two Ca^{2+} cations are surrounded by eight (Ca1) and nine (Ca2) O atoms, considering a cut-off value of 3.1 Å for relevant Ca—O distances (Table 1). The bond valence sums (Brown, 2002) computed with the parameters of Brown & Altermatt (1985) are 1.89 valence units (v.u.) for Ca1 and 2.02 v.u. for Ca2, in good agreement with the expected value of 2. Likewise, the mean Ca—O bond length of 2.55 Å for Ca1 and 2.57 Å for Ca2 are in accord with the values for eight- and nine-coordinate Ca of 2.50 (15) and 2.56 (20) Å, respectively (Gagné & Hawthorne, 2016). Whereas the $[Ca1O_8]$ polyhedron is difficult to derive from a simple geometric figure, $[Ca2O_9]$ can be best described as a monocapped square antiprism (Fig. 1).

All four Te atoms have an oxidation state of +IV and can be divided into two pairs with the most commonly observed three-coordination in the form of a trigonal pyramid (Te2 and Te4) and four-coordination in the form of a bisphenoid (Te1 and Te3). The Te—O bond lengths within the $[TeO_3]$ trigonal pyramids are only slightly spread, ranging from 1.8522 (12) to 1.8994 (11) Å. The two $[TeO_4]$ bisphenoids are characterised by two short bonds of < 2 Å and two longer bonds of > 2 Å, with the maximum at 2.3222 (12) Å for Te3. All Te—O bond lengths (Table 1) are in characteristic ranges for oxotellurates(IV) with three- and four-coordinate tellurium, as reviewed recently by Christy *et al.* (2016).

Bond valence sums for the four Te atoms computed with the parameters of Brese and O'Keeffe (1991) are 4.14, 4.07, 3.99 and 3.81 v.u., but are considerably lower when the revised parameters of Mills & Christy (2013) are used, *i.e.* 3.93, 3.80, 3.81 and 3.57 v.u.

The oxotellurium(IV) network is built up from two different anions, both with composition $[Te_3O_8]^{4-}$. One anion is made up from an infinite zigzag chain that extends parallel to [001] and consists of a pair of corner-sharing $[Te3O_4]$ bisphenoids linked alternately to a $[Te4O_3]$ trigonal pyramid {= $[(Te4O_{1/1}O_{2/2})(Te3O_{2/1}O_{2/2})_2]_n$} (Fig. 2*a*). The second oxotellurate(IV) anion is finite and is situated between neighbouring chain anions. It is comprised of a curved $[Te_3O_8]^{4-}$ unit with a

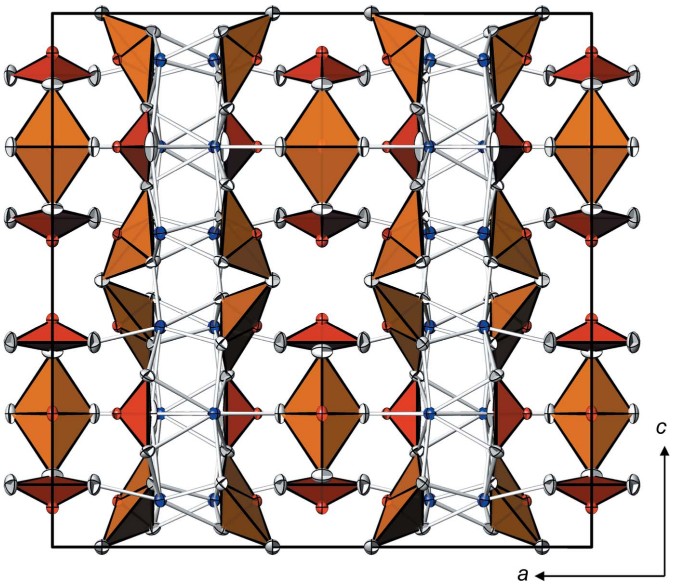


Figure 3
The crystal structure of $Ca_2Te_3O_8$ in a projection along $[0\bar{1}0]$. Displacement ellipsoids and colour code as in Figs. 1 and 2.

central $Te1O_4$ bisphenoid linked to two $[Te2O_3]$ trigonal pyramids $\{= [(Te1O_{2/1}O_{1/2})_2(Te2O_{2/2}O_{2/1})]\}$ (Fig. 2*b*).

In the crystal, the two types of $[Te_3O_8]^{4-}$ anions are arranged in layers parallel to (100). Approximately at $x \simeq 1/4$ and 3/4, the calcium cations link adjacent layers into the three-dimensional framework (Fig. 3).

Table 2
Experimental details.

Crystal data	
Chemical formula	$Ca_2Te_3O_8$
M_r	590.95
Crystal system, space group	Orthorhombic, *Cmcm*
Temperature (K)	297
a, b, c (Å)	18.7368 (15), 6.8399 (6), 18.5652 (15)
V (Å^3)	2379.3 (3)
Z	12
Radiation type	Mo $K\alpha$
μ (mm^{-1})	12.27
Crystal size (mm)	0.25 × 0.15 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.472, 0.750
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	47523, 6097, 5325
R_{int}	0.043
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	1.057
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.023, 0.043, 1.12
No. of reflections	6097
No. of parameters	101
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	4.13, −2.08

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXL2017* (Sheldrick, 2015), *ATOMS* (Dowty, 2006) and *publCIF* (Westrip, 2010). Starting coordinates taken from an isotypic compound.

$Ca_2Te_3O_8$ is isotypic with $Pb_2Te_3O_8$ (Champarnaud-Mesjard *et al.*, 2001), but not with its higher alkaline earth homologue $Sr_2Te_3O_8$, which is reported to have a different orthorhombic cell, with details of the structure not known (Elerman & Koçak, 1986). Comparison of the bond lengths of the $[MO_x]$ (M = Ca, Pb) polyhedra and the $[TeO_3]$ and $[TeO_4]$ units in the isotypic structures of $Ca_2Te_3O_8$ and $Pb_2Te_3O_8$ (Table 1) reveals nearly identical values for the individual oxotellurate(IV) units, but differences up to 0.6 Å for the metal–oxygen polyhedra. On one hand, this behaviour is ascribed to the different ionic radii for eight-coordinate Ca^{II} and Pb^{II} of 1.12 and 1.29 Å, respectively (Shannon, 1976), and, on the other hand, to the stereochemical activity (Galy *et al.*, 1975) of the $6s^2$ free-electron lone pair located at Pb^{II} that is responsible for the formation of off-centred lead–oxygen polyhedra with either holo- or hemidirected oxygen ligands (Shimoni-Livny *et al.*, 1998).

For a quantitative structural comparison of the isotypic $M_2Te_3O_8$ (M = Ca, Pb) structures, 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 0.0205, the maximum distance between the atomic positions of paired atoms is 0.403 Å for pair O8, the arithmetic mean of all distances is 0.195 Å and the measure of similarity is 0.05.

3. Synthesis and crystallization

Crystals of $Ca_2Te_3O_8$ were obtained as one of the products from a flux synthesis using a CsCl/NaCl salt mixture (molar ratio 0.65/0.35). To 1.5 g of the salt mixture were added CaO (0.075 g; freshly prepared by heating $CaCO_3$ at 1473 K for 1 d) and TeO_2 (0.425 g) according to a molar ratio of 1:2. The reaction mixture was placed in a silica ampoule that was subsequently evacuated and sealed. The ampoule was placed vertically in a furnace and heated from room temperature within 3 h to 793 K, kept at that temperature for 90 h and cooled within 10 h to room temperature. The silica ampoule was broken and the solidified melt leached out with water for two h. The colourless product was filtered off, washed with water and was dried in a stream of air. The title compound was present in the form of a few crystals that were distinguishable from the other crystals due to their characteristic square form (maximum edge length 1.5 mm). Other phases identified by single-crystal X-ray diffraction measurements of selected crystals and by powder X-ray diffraction measurements of the bulk were $CaTe_2O_5$ in the mica-like modification reported by Redman *et al.* (1970) as the main phase (tiny colourless plates) and $Ca_4Te_5O_{14}$ (small colourless pinacoids; Weil, 2004).

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Starting coordinates for the refinement were taken from isotypic $Pb_2Te_3O_8$ (Champarnaud-Mesjard *et al.*, 2001). Both remaining maximum and minimum electron-density peaks are located 0.64 and 0.30 Å from the Te2 site.

Acknowledgements

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$Ca_2Te_3O_8$, a new phase in the CaO–TeO_2 system

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: coordinates from isotypic compound; program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015); molecular graphics: *ATOMS* (Dowty, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Dicalcium octaoxidotritellurate(IV)

Crystal data

$Ca_2Te_3O_8$
$M_r = 590.95$
Orthorhombic, *Cmcm*
$a = 18.7368\ (15)$ Å
$b = 6.8399\ (6)$ Å
$c = 18.5652\ (15)$ Å
$V = 2379.3\ (3)$ Å^3
$Z = 12$
$F(000) = 3120$
$D_x = 4.949$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9248 reflections
$\theta = 3.2–48.6°$
$\mu = 12.27$ mm^{-1}
$T = 297$ K
Plate, colourless
0.25 × 0.15 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
$T_{min} = 0.472$, $T_{max} = 0.750$
47523 measured reflections
6097 independent reflections
5325 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 48.7°$, $\theta_{min} = 2.2°$
$h = -37\rightarrow39$
$k = -14\rightarrow14$
$l = -36\rightarrow39$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.043$
$S = 1.12$
6097 reflections
101 parameters
0 restraints
Primary atom site location: isomorphous structure methods
$w = 1/[\sigma^2(F_o^2) + (0.0102P)^2 + 6.3377P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 4.13$ e Å^{-3}
$\Delta\rho_{min} = -2.08$ e Å^{-3}
Extinction correction: SHELXL2017 (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00143 (3)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ca1	0.29994 (2)	0.36584 (4)	0.41210 (2)	0.00884 (4)
Ca2	0.19996 (2)	0.49754 (6)	0.250000	0.00819 (5)
Te1	0.500000	0.08952 (3)	0.250000	0.00866 (3)
Te2	0.500000	0.29743 (2)	0.07448 (2)	0.00865 (2)
Te3	0.37898 (2)	0.84140 (2)	0.41362 (2)	0.00685 (2)
Te4	0.37986 (2)	0.54478 (2)	0.250000	0.00616 (2)
O1	0.500000	0.0728 (2)	0.13377 (9)	0.0150 (3)
O2	0.40826 (9)	0.000000	0.500000	0.0146 (3)
O3	0.31332 (6)	0.69421 (16)	0.46567 (6)	0.01057 (16)
O4	0.32340 (7)	0.67071 (18)	0.32118 (6)	0.01226 (17)
O5	0.31362 (6)	0.02866 (15)	0.38074 (6)	0.00918 (15)
O6	0.42263 (7)	0.42092 (19)	0.11674 (8)	0.0165 (2)
O7	0.42329 (9)	0.9223 (3)	0.250000	0.0135 (3)
O8	0.31736 (10)	0.3318 (3)	0.250000	0.0209 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.00841 (9)	0.00807 (9)	0.01005 (9)	0.00102 (7)	−0.00031 (7)	0.00024 (7)
Ca2	0.00857 (13)	0.00778 (12)	0.00821 (12)	0.00113 (10)	0.000	0.000
Te1	0.00648 (6)	0.00643 (6)	0.01305 (7)	0.000	0.000	0.000
Te2	0.00773 (4)	0.00848 (4)	0.00974 (4)	0.000	0.000	−0.00001 (3)
Te3	0.00550 (3)	0.00710 (3)	0.00794 (3)	0.00067 (2)	0.00072 (2)	0.00095 (2)
Te4	0.00569 (4)	0.00572 (4)	0.00706 (4)	0.00012 (3)	0.000	0.000
O1	0.0227 (8)	0.0108 (6)	0.0116 (6)	0.000	0.000	0.0018 (5)
O2	0.0110 (6)	0.0209 (7)	0.0119 (6)	0.000	0.000	−0.0089 (5)
O3	0.0123 (4)	0.0103 (4)	0.0091 (4)	−0.0023 (3)	0.0028 (3)	0.0010 (3)
O4	0.0122 (4)	0.0157 (4)	0.0088 (4)	0.0031 (3)	0.0022 (3)	−0.0022 (3)
O5	0.0096 (4)	0.0072 (3)	0.0107 (4)	0.0021 (3)	−0.0006 (3)	0.0000 (3)
O6	0.0091 (4)	0.0175 (5)	0.0228 (6)	0.0037 (4)	0.0000 (4)	−0.0049 (4)
O7	0.0072 (5)	0.0142 (6)	0.0193 (7)	−0.0022 (5)	0.000	0.000
O8	0.0099 (7)	0.0077 (6)	0.0451 (12)	−0.0030 (5)	0.000	0.000

Geometric parameters (Å, º)

Ca1—O3^{i}	2.3198 (11)	Ca2—O4	2.9154 (13)
Ca1—O6^{ii}	2.3903 (13)	Ca2—O4^{ii}	2.9154 (13)
Ca1—O5	2.3924 (11)	Ca2—Te4	3.3863 (5)
Ca1—O3	2.4691 (12)	Ca2—Te4^{vi}	3.4390 (5)

Ca1—O5^{iii}	2.4712 (11)	Ca2—Te3^{vi}	3.5434 (3)
Ca1—O3^{iv}	2.6212 (12)	Te1—O7^{vii}	1.8369 (17)
Ca1—O4	2.7186 (13)	Te1—O7^{viii}	1.8369 (17)
Ca1—O8	3.0360 (4)	Te1—O1	2.1608 (17)
Ca1—Te3^{iv}	3.3567 (4)	Te1—O1^{ii}	2.1609 (17)
Ca1—Te3	3.5742 (4)	Te2—O6^{ix}	1.8522 (12)
Ca1—Te4	3.5773 (4)	Te2—O6	1.8522 (12)
Ca1—Ca2	3.6575 (4)	Te2—O1	1.8902 (17)
Ca2—O8^{v}	2.3089 (18)	Te3—O3	1.8602 (11)
Ca2—O7^{vi}	2.3660 (17)	Te3—O5^{x}	1.8743 (10)
Ca2—O5^{v}	2.4497 (11)	Te3—O2^{x}	2.0123 (5)
Ca2—O5^{iii}	2.4497 (11)	Te3—O4	2.3222 (12)
Ca2—O8	2.4749 (19)	Te4—O8	1.8694 (17)
Ca2—O4^{vi}	2.6335 (13)	Te4—O4	1.8994 (11)
Ca2—O4^{iv}	2.6335 (13)	Te4—O4^{ii}	1.8994 (11)

O3^{i}—Ca1—O6^{ii}	98.22 (5)	O8^{v}—Ca2—Te3^{vi}	103.87 (2)
O3^{i}—Ca1—O5	93.20 (4)	O7^{vi}—Ca2—Te3^{vi}	61.771 (12)
O6^{ii}—Ca1—O5	89.68 (4)	O5^{v}—Ca2—Te3^{vi}	29.94 (2)
O3^{i}—Ca1—O3	75.88 (4)	O5^{iii}—Ca2—Te3^{vi}	146.33 (3)
O6^{ii}—Ca1—O3	81.32 (4)	O8—Ca2—Te3^{vi}	103.47 (2)
O5—Ca1—O3	164.59 (4)	O4^{vi}—Ca2—Te3^{vi}	40.94 (3)
O3^{i}—Ca1—O5^{iii}	113.79 (4)	O4^{iv}—Ca2—Te3^{vi}	96.03 (3)
O6^{ii}—Ca1—O5^{iii}	134.77 (4)	O4—Ca2—Te3^{vi}	147.38 (2)
O5—Ca1—O5^{iii}	117.99 (4)	O4^{ii}—Ca2—Te3^{vi}	93.73 (2)
O3—Ca1—O5^{iii}	76.84 (4)	Te4—Ca2—Te3^{vi}	116.377 (7)
O3^{i}—Ca1—O3^{iv}	68.72 (4)	Te4^{vi}—Ca2—Te3^{vi}	63.068 (6)
O6^{ii}—Ca1—O3^{iv}	159.11 (4)	O7^{vii}—Te1—O7^{viii}	102.97 (11)
O5—Ca1—O3^{iv}	75.37 (4)	O7^{vii}—Te1—O1	88.11 (3)
O3—Ca1—O3^{iv}	109.69 (4)	O7^{viii}—Te1—O1	88.11 (3)
O5^{iii}—Ca1—O3^{iv}	66.05 (4)	O7^{vii}—Te1—O1^{ii}	88.11 (3)
O3^{i}—Ca1—O4	136.52 (4)	O7^{viii}—Te1—O1^{ii}	88.11 (3)
O6^{ii}—Ca1—O4	65.45 (4)	O1—Te1—O1^{ii}	173.92 (9)
O5—Ca1—O4	124.82 (4)	O7^{vii}—Te1—Ca2^{vi}	28.98 (5)
O3—Ca1—O4	62.35 (4)	O7^{viii}—Te1—Ca2^{vi}	131.95 (6)
O5^{iii}—Ca1—O4	69.34 (4)	O1—Te1—Ca2^{vi}	89.497 (8)
O3^{iv}—Ca1—O4	135.24 (4)	O1^{ii}—Te1—Ca2^{vi}	89.497 (8)
O3^{i}—Ca1—O8	160.81 (5)	O7^{vii}—Te1—Ca2^{xi}	131.95 (6)
O6^{ii}—Ca1—O8	71.74 (5)	O7^{viii}—Te1—Ca2^{xi}	28.98 (5)
O5—Ca1—O8	70.93 (4)	O1—Te1—Ca2^{xi}	89.497 (8)
O3—Ca1—O8	117.27 (4)	O1^{ii}—Te1—Ca2^{xi}	89.497 (8)
O5^{iii}—Ca1—O8	83.89 (4)	Ca2^{vi}—Te1—Ca2^{xi}	160.934 (13)
O3^{iv}—Ca1—O8	115.39 (4)	O6^{ix}—Te2—O6	103.01 (8)
O4—Ca1—O8	54.98 (4)	O6^{ix}—Te2—O1	97.12 (6)
O3^{i}—Ca1—Te3^{iv}	95.22 (3)	O6—Te2—O1	97.12 (6)
O6^{ii}—Ca1—Te3^{iv}	165.99 (3)	O6^{ix}—Te2—Ca1^{xii}	30.77 (4)
O5—Ca1—Te3^{iv}	93.50 (3)	O6—Te2—Ca1^{xii}	133.69 (4)
O3—Ca1—Te3^{iv}	98.24 (3)	O1—Te2—Ca1^{xii}	93.563 (8)

O5^{iii}—Ca1—Te3^{iv}	33.33 (2)	O6^{ix}—Te2—Ca1^{ii}	133.69 (4)
O3^{iv}—Ca1—Te3^{iv}	33.48 (2)	O6—Te2—Ca1^{ii}	30.77 (4)
O4—Ca1—Te3^{iv}	101.83 (3)	O1—Te2—Ca1^{ii}	93.563 (8)
O8—Ca1—Te3^{iv}	96.42 (4)	Ca1^{xii}—Te2—Ca1^{ii}	163.902 (10)
O3^{i}—Ca1—Te3	96.23 (3)	O3—Te3—O5^{x}	96.14 (5)
O6^{ii}—Ca1—Te3	57.30 (3)	O3—Te3—O2^{x}	93.33 (5)
O5—Ca1—Te3	146.60 (3)	O5^{x}—Te3—O2^{x}	93.97 (5)
O3—Ca1—Te3	29.18 (3)	O3—Te3—O4	79.35 (5)
O5^{iii}—Ca1—Te3	87.05 (3)	O5^{x}—Te3—O4	79.04 (5)
O3^{iv}—Ca1—Te3	137.74 (3)	O2^{x}—Te3—O4	169.18 (6)
O4—Ca1—Te3	40.52 (3)	O3—Te3—Ca1^{iii}	51.01 (4)
O8—Ca1—Te3	91.90 (3)	O5^{x}—Te3—Ca1^{iii}	46.42 (3)
Te3^{iv}—Ca1—Te3	117.328 (9)	O2^{x}—Te3—Ca1^{iii}	104.60 (5)
O3^{i}—Ca1—Te4	146.96 (3)	O4—Te3—Ca1^{iii}	64.59 (3)
O6^{ii}—Ca1—Te4	49.84 (3)	O3—Te3—Ca2^{v}	109.41 (4)
O5—Ca1—Te4	94.60 (3)	O5^{x}—Te3—Ca2^{v}	40.72 (3)
O3—Ca1—Te4	89.14 (3)	O2^{x}—Te3—Ca2^{v}	129.382 (18)
O5^{iii}—Ca1—Te4	90.46 (3)	O4—Te3—Ca2^{v}	47.99 (3)
O3^{iv}—Ca1—Te4	144.22 (3)	Ca1^{iii}—Te3—Ca2^{v}	63.955 (8)
O4—Ca1—Te4	31.52 (2)	O3—Te3—Ca1	40.32 (4)
O8—Ca1—Te4	31.50 (3)	O5^{x}—Te3—Ca1	110.40 (3)
Te3^{iv}—Ca1—Te4	116.244 (9)	O2^{x}—Te3—Ca1	127.580 (17)
Te3—Ca1—Te4	61.433 (6)	O4—Te3—Ca1	49.52 (3)
O3^{i}—Ca1—Ca2	154.68 (3)	Ca1^{iii}—Te3—Ca1	68.372 (6)
O6^{ii}—Ca1—Ca2	105.63 (3)	Ca2^{v}—Te3—Ca1	95.427 (9)
O5—Ca1—Ca2	95.28 (3)	O3—Te3—Ca1^{i}	26.53 (4)
O3—Ca1—Ca2	99.17 (3)	O5^{x}—Te3—Ca1^{i}	105.99 (3)
O5^{iii}—Ca1—Ca2	41.77 (3)	O2^{x}—Te3—Ca1^{i}	68.39 (3)
O3^{iv}—Ca1—Ca2	90.45 (3)	O4—Te3—Ca1^{i}	105.36 (3)
O4—Ca1—Ca2	51.91 (3)	Ca1^{iii}—Te3—Ca1^{i}	68.861 (8)
O8—Ca1—Ca2	42.13 (4)	Ca2^{v}—Te3—Ca1^{i}	132.402 (9)
Te3^{iv}—Ca1—Ca2	60.505 (8)	Ca1—Te3—Ca1^{i}	60.638 (8)
Te3—Ca1—Ca2	89.690 (9)	O8—Te4—O4	90.26 (6)
Te4—Ca1—Ca2	55.803 (9)	O8—Te4—O4^{ii}	90.26 (6)
O8^{v}—Ca2—O7^{vi}	94.49 (6)	O4—Te4—O4^{ii}	88.18 (7)
O8^{v}—Ca2—O5^{v}	84.22 (3)	O8—Te4—Ca2	45.74 (6)
O7^{vi}—Ca2—O5^{v}	85.27 (3)	O4—Te4—Ca2	59.26 (4)
O8^{v}—Ca2—O5^{iii}	84.22 (3)	O4^{ii}—Te4—Ca2	59.26 (4)
O7^{vi}—Ca2—O5^{iii}	85.27 (3)	O8—Te4—Ca2^{v}	115.43 (6)
O5^{v}—Ca2—O5^{iii}	164.44 (5)	O4—Te4—Ca2^{v}	49.41 (4)
O8^{v}—Ca2—O8	125.35 (5)	O4^{ii}—Te4—Ca2^{v}	49.42 (4)
O7^{vi}—Ca2—O8	140.16 (6)	Ca2—Te4—Ca2^{v}	69.699 (8)
O5^{v}—Ca2—O8	97.59 (3)	O8—Te4—Ca1	58.067 (9)
O5^{iii}—Ca2—O8	97.59 (3)	O4—Te4—Ca1	48.45 (4)
O8^{v}—Ca2—O4^{vi}	144.79 (4)	O4^{ii}—Te4—Ca1	120.49 (4)
O7^{vi}—Ca2—O4^{vi}	69.70 (5)	Ca2—Te4—Ca1	63.297 (6)
O5^{v}—Ca2—O4^{vi}	63.85 (3)	Ca2^{v}—Te4—Ca1	97.242 (7)
O5^{iii}—Ca2—O4^{vi}	123.62 (4)	O8—Te4—Ca1^{ii}	58.067 (9)

O8—Ca2—O4^{vi}	76.04 (5)
O8^{v}—Ca2—O4^{iv}	144.79 (4)
O7^{vi}—Ca2—O4^{iv}	69.70 (5)
O5^{v}—Ca2—O4^{iv}	123.62 (4)
O5^{iii}—Ca2—O4^{iv}	63.85 (3)
O8—Ca2—O4^{iv}	76.04 (5)
O4^{vi}—Ca2—O4^{iv}	60.24 (5)
O8^{v}—Ca2—O4	73.10 (5)
O7^{vi}—Ca2—O4	149.63 (3)
O5^{v}—Ca2—O4	119.75 (4)
O5^{iii}—Ca2—O4	66.29 (3)
O8—Ca2—O4	58.73 (4)
O4^{vi}—Ca2—O4	134.77 (3)
O4^{iv}—Ca2—O4	104.43 (4)
O8^{v}—Ca2—O4^{ii}	73.10 (5)
O7^{vi}—Ca2—O4^{ii}	149.63 (3)
O5^{v}—Ca2—O4^{ii}	66.29 (3)
O5^{iii}—Ca2—O4^{ii}	119.75 (4)
O8—Ca2—O4^{ii}	58.73 (4)
O4^{vi}—Ca2—O4^{ii}	104.43 (4)
O4^{iv}—Ca2—O4^{ii}	134.77 (3)
O4—Ca2—O4^{ii}	53.91 (5)
O8^{v}—Ca2—Te4	92.60 (5)
O7^{vi}—Ca2—Te4	172.91 (4)
O5^{v}—Ca2—Te4	95.46 (3)
O5^{iii}—Ca2—Te4	95.46 (3)
O8—Ca2—Te4	32.75 (4)
O4^{vi}—Ca2—Te4	104.27 (3)
O4^{iv}—Ca2—Te4	104.27 (3)
O4—Ca2—Te4	34.05 (2)
O4^{ii}—Ca2—Te4	34.05 (2)
O8^{v}—Ca2—Te4^{vi}	146.15 (5)
O7^{vi}—Ca2—Te4^{vi}	51.66 (4)
O5^{v}—Ca2—Te4^{vi}	91.90 (3)
O5^{iii}—Ca2—Te4^{vi}	91.90 (3)
O8—Ca2—Te4^{vi}	88.51 (4)
O4^{vi}—Ca2—Te4^{vi}	33.21 (2)
O4^{iv}—Ca2—Te4^{vi}	33.21 (2)
O4—Ca2—Te4^{vi}	135.31 (3)
O4^{ii}—Ca2—Te4^{vi}	135.31 (3)
Te4—Ca2—Te4^{vi}	121.252 (12)
O4—Te4—Ca1^{ii}	120.49 (4)
O4^{ii}—Te4—Ca1^{ii}	48.45 (4)
Ca2—Te4—Ca1^{ii}	63.299 (6)
Ca2^{v}—Te4—Ca1^{ii}	97.242 (7)
Ca1—Te4—Ca1^{ii}	114.545 (11)
Te2—O1—Te1	122.58 (9)
Te3^{vii}—O2—Te3^{i}	148.36 (9)
Te3—O3—Ca1^{i}	132.49 (6)
Te3—O3—Ca1	110.51 (5)
Ca1^{i}—O3—Ca1	102.82 (4)
Te3—O3—Ca1^{iii}	95.51 (5)
Ca1^{i}—O3—Ca1^{iii}	111.28 (4)
Ca1—O3—Ca1^{iii}	99.92 (4)
Te4—O4—Te3	119.50 (6)
Te4—O4—Ca2^{v}	97.37 (5)
Te3—O4—Ca2^{v}	91.07 (4)
Te4—O4—Ca1	100.03 (5)
Te3—O4—Ca1	89.96 (4)
Ca2^{v}—O4—Ca1	159.36 (5)
Te4—O4—Ca2	86.69 (4)
Te3—O4—Ca2	153.51 (5)
Ca2^{v}—O4—Ca2	89.17 (4)
Ca1—O4—Ca2	80.88 (3)
Te3^{vii}—O5—Ca1	130.51 (5)
Te3^{vii}—O5—Ca2^{vi}	109.34 (5)
Ca1—O5—Ca2^{vi}	108.29 (4)
Te3^{vii}—O5—Ca1^{iv}	100.25 (5)
Ca1—O5—Ca1^{iv}	106.55 (4)
Ca2^{vi}—O5—Ca1^{iv}	96.02 (4)
Te2—O6—Ca1^{ii}	125.87 (7)
Te1^{x}—O7—Ca2^{v}	128.92 (9)
Te4—O8—Ca2^{vi}	149.29 (10)
Te4—O8—Ca2	101.52 (8)
Ca2^{vi}—O8—Ca2	109.19 (7)
Te4—O8—Ca1	90.43 (3)
Ca2^{vi}—O8—Ca1	93.49 (3)
Ca2—O8—Ca1	82.49 (4)
Te4—O8—Ca1^{ii}	90.43 (3)
Ca2^{vi}—O8—Ca1^{ii}	93.49 (3)
Ca2—O8—Ca1^{ii}	82.49 (4)
Ca1—O8—Ca1^{ii}	164.82 (7)

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