



Crystal structures of the triple perovskites $\text{Ba}_2\text{K}_2\text{Te}_2\text{O}_9$ and $\text{Ba}_2\text{KNaTe}_2\text{O}_9$, and redetermination of the double perovskite $\text{Ba}_2\text{CaTeO}_6$

Matthias Weil*

Received 13 June 2018
Accepted 21 June 2018

Institute for Chemical Technologies and Analytics, Division of Structural Chemistry, TU Wien, Getreidemarkt 9/164-SC, A-1060 Vienna, Austria. *Correspondence e-mail: matthias.weil@tuwien.ac.at

Edited by T. J. Prior, University of Hull, England

Keywords: crystal structure; perovskite family; $6H\text{-BaTiO}_3$ structure type; double perovskite; isotypism.

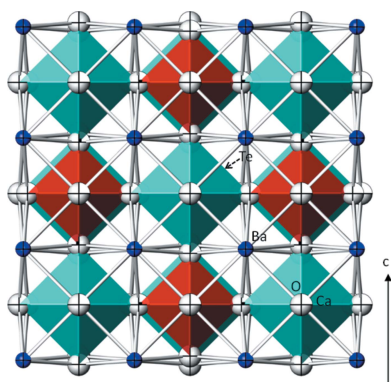
CCDC references: 1850819; 1850818; 1850817

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

Single crystals of $\text{Ba}_2\text{K}_2\text{Te}_2\text{O}_9$ (dibarium dipotassium nonaoxidoditellurate), (I), $\text{Ba}_2\text{KNaTe}_2\text{O}_9$ (dibarium potassium sodium nonaoxidoditellurate), (II), and $\text{Ba}_2\text{CaTeO}_6$ (dibarium calcium hexaoxidotellurate), (III), were obtained from KNO_3/KI or $\text{KNO}_3/\text{NaNO}_3$ flux syntheses in platinum crucibles for (I) and (II), or porcelain crucibles for (III). (I) and (II) are isotypic and are members of triple perovskites with general formula $A_2^{[12co]}A'^{[12co]}B_2^{[6o]}B'^{[6o]}\text{O}_9$. They crystallize in the $6H\text{-BaTiO}_3$ structure family in space-group type $P6_3/mmc$, with the A, A', B and B' sites being occupied by K, Ba, Te and a second Ba in (I), and in (II) by mixed-occupied (Ba/K), Ba, Te and Na sites, respectively. (III) adopts the $A_2^{[12co]}B'^{[6o]}B''^{[6o]}\text{O}_6$ double perovskite structure in space-group type $Fm\bar{3}m$, with Ba, Ca and Te located on the A, B' and B'' sites, respectively. The current refinement of (III) is based on single-crystal X-ray data. It confirms the previous refinement from X-ray powder diffraction data [Fu *et al.* (2008). *J. Solid State Chem.* **181**, 2523–2529], but with higher precision.

1. Chemical context

During a recent project on the structure determination of barium oxotellurates(VI), different preparation methods were applied for single-crystal growth of the phases $\text{Ba}[\text{H}_4\text{TeO}_6]$, $\text{Ba}[\text{H}_2\text{TeO}_5]$, $\text{Ba}[\text{Te}_2\text{O}_6(\text{OH})_2]$ and $\text{Ba}[\text{TeO}_4]$ (Weil *et al.*, 2016). Owing to the different water content that defines the thermal stability range of the respective phase, relatively mild temperatures < 600 K had to be adjusted for the three hydrous phases using either a diffusion method in aqueous solutions (room temperature) or hydrothermal methods (*ca* 470 K), whereas for the anhydrous phase higher temperatures could be employed. However, $\text{Ba}[\text{TeO}_4]$ decomposes into $\text{Ba}[\text{TeO}_3]$ with release of oxygen at temperatures above 1000 K, which prevents prolonged heating near this temperature. Although very small crystals of $\text{Ba}[\text{TeO}_4]$ with a rather poor quality could eventually be grown by heating $\text{Ba}[\text{H}_4\text{TeO}_6]$ at 873 K for some days (Weil *et al.*, 2016), alternative crystal-growth methods were tested with the intention of obtaining larger crystals with better quality. With the upper stability range of the target phase $\text{Ba}[\text{TeO}_4]$ in mind, KNO_3/KI or $\text{KNO}_3/\text{NaNO}_3$ mixtures were used for crystal-growth experiments. Such salt mixtures have low eutectic melting points, *e.g.* 498 K for a 50:50 mol% mixture of $\text{NaNO}_3/\text{KNO}_3$ (Berg & Kerridge, 2004). At least for the latter eutectic mixture, crystal-growth experiments from the melt have already been applied successfully for another barium phase, *viz.* $\text{Ba}_2\text{As}_2\text{O}_7$ (Weil,



OPEN ACCESS

2016). However, Ba[TeO₄] did not form under the given conditions because K⁺ or mixtures of K⁺ and Na⁺ were incorporated instead, resulting in the formation of Ba₂K₂Te₂O₉ (I) or Ba₂KNaTe₂O₉ (II) single crystals. In the case a porcelain crucible was employed, Ba₂CaTeO₆ (III) was obtained in form of very few single crystals.

2. Structural commentary

The three title compounds belong to the vast family of perovskites (Tilley, 2016). The ideal cubic $A^{[12co]}B^{[6o]}O_3$ perovskite structure comprises of corner-sharing [BO₆] octahedra. In the centre of the resulting $\infty^3[BO_{6/2}]$ network, the A-site cation occupies a 12-coordinate cuboctahedral site. The 2H hexagonal perovskite structure contains chains of face-sharing [BO₆] octahedra that are separated by chains of A-site cations. In an alternative description, perovskite structures can be derived from closed-packed arrangements of the anions with different stacking sequences (Lufaso & zur Loye, 2005a; Stöger *et al.*, 2010). For example, in the cubic perovskite an ABC stacking and in the hexagonal 2H perovskite an AB stacking is observed. More complex structures that are realized in double perovskites or triple perovskites can include both cubic (*c*) and hexagonal stacking sequences (*h*) and consequently structure motifs of corner-sharing and face-sharing [BO₆] octahedra like in the triple perovskites discussed below.

Ba₂K₂Te₂O₉ (I) and Ba₂KNaTe₂O₉ (II) are isotypic and members of the triple perovskite family with general formula $A_2^{[12co]}A'^{[12co]}B_2^{[6o]}B'^{[6o]}O_9$. They crystallize in the 6H-BaTiO₃ structure type in space-group type $P6_3/mmc$ with $Z = 2$. In (I) the A, A', B and B' sites are occupied by K1, Ba1, Te1 and Ba2, and in (II) by mixed-occupied (Ba/K)1, Ba1, Te1 and Na2, respectively. The 6H-BaTiO₃ structure type is sometimes also referred to as the BaFeO_{2+x} structure type with possible values for $Z = 2, 3$ or 6, dependent on the overall formula sum of the compound. The stacking sequence for this structure type is (cch)₂ (Tilley, 2016). About 240 entries of this structure family are compiled in the recent version of the Inorganic Crystal Structure Database (ICSD, 2018), with hexagonal BaTiO₃ being the first phase that has been structurally determined (Burbank & Evans, 1948). Only four Te-containing phases have been reported so far to adopt this structure type, *viz.* Ba₃Fe₂TeO₉ (Harari *et al.*, 1972), K₃LaTe₂O₉ (Zhang *et al.*, 2015), Ba₃Cr_{1.94}Te_{1.06}O₉ (Li *et al.*, 2016) and the high-pressure phase Ba₂NiTeO₆ ($Z = 3$; Aoba *et al.*, 2016). A review of this structure type and of perovskites in general was given recently by Tilley (2016). In both structures (I) and (II), Ba1 is situated on Wyckoff position 2b (site symmetry $\bar{6}m2$), the K1 site in (I) and the mixed-occupied (Ba/K)1 site (occupancy ratio 1:1) in (II) on 4f ($3m.$), Ba2 in (I) and Na2 in (II) on 2a ($\bar{3}m.$), and in both structures Te1 4f ($3m.$), O1 on 6h ($mm2$) and O2 on 12k ($m.$), respectively. Hence the smaller Te^{VI} atoms occupy the face-sharing octahedral B site while the larger barium (Ba2 in (I)) or sodium cations (Na2 in (II)) occupy the corner-sharing octahedral B' site. The inner angles of the two face-sharing [TeO₆] octahedra in (I) and (II) (Table 1) are more similar

than those in isotypic triple perovskites (Lufaso & zur Loye, 2005a), with center shifts of 0.076 Å in (I) and of 0.191 Å in (II). Representative for both (I) and (II), the crystal structure of Ba₂K₂Te₂O₉ is given in Fig. 1. It should be noted that the A (= K1) position in (I) has only nine coordination partners, while in (II) twelve oxygen atoms surround the corresponding site that is statistically occupied by Ba²⁺ and K⁺ (= (Ba/K)1).

The current refinement of Ba₂CaTeO₆ (III) is based on single crystal X-ray data and confirms the previous structure determination from X-ray powder diffraction data, but with higher precision (reliability factors for the previous determination: $R_{wp} = 0.159$, $R_p = 0.112$; Fu *et al.*, 2008). Ba₂CaTeO₆ (III) is a member of the double perovskite family with general formula $A_2^{[12co]}B^{[6o]}B'^{[6o]}O_6$. Dependent on the cations

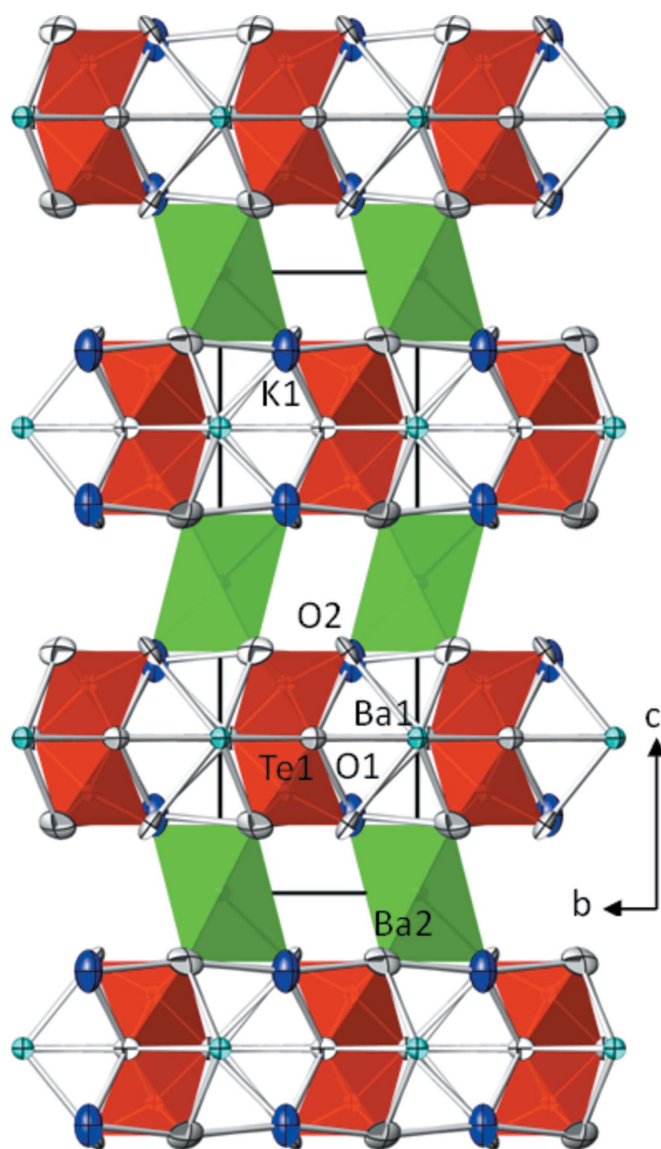


Figure 1
Projection of the crystal structure of Ba₂K₂Te₂O₉ (I) along $[\bar{1}00]$. [Ba₂O₆] octahedra are green, [TeO₆] octahedra are red, potassium sites are blue, Ba1 sites turquoise and O sites shaded pale grey. Displacement ellipsoids are drawn at the 97% probability level.

Table 1
Selected bond lengths (Å) and angles (°) in the structures (I)–(III).

(I)		(II)		(III)	
K1–O1	2.893 (2) [3×]	(Ba/K)1–O2	2.98780 (19) [6×]	Ba–O	2.9577 (5) [12×]
K1–O2	3.0359 (17) [6×]	(Ba/K)1–O2	3.1064 (19) [3×]	Ca–O	2.247 (3) [6×]
		(Ba/K)1–O1	3.1927 (12) [3×]	Te–O	1.930 (3) [6×]
Ba1–O2	2.952 (2) [6×]	Ba1–O2	2.9532 (18) [6×]		
Ba1–O1	3.0382 (17) [6×]	Ba1–O1	2.9935 (14) [6×]		
Te1–O2	1.8524 (18) [3×]	Te1–O2	1.8481 (16) [3×]		
Te1–O1	2.0474 (16) [3×]	Te1–O1	2.0418 (14) [3×]		
Ba2–O2	2.5910 (18) [6×]	Na2–O2	2.3037 (16) [6×]		
O1–Te1–O1	75.43 (7) [3×]	O1–Te1–O1	75.95 (6) [3×]		
Δ^a	0.076	Δ^a	0.191		

Note: (a) Δ is the center shift (Å) of the Te atoms in the Te_2O_9 dimer. The center shift is defined as the distance between the Te atoms in the 4f Wyckoff position ($z \approx 1/6$) of the actual crystal structure and the ideal high-symmetry 4f Te position ($z = 1/6$) (Lufaso & zur Loye, 2005a).

present at the B' and B'' sites, double perovskites are functional oxide materials with interesting electronic and magnetic properties (Vasala & Karppinen, 2015). In the crystal structure of (III), Ba, Ca and Te are located on the A , B' and B'' sites, respectively. The Wyckoff positions and site symmetries of the four sites present in the structure of (III) are: Ba on $8c$ ($4\bar{3}m$), Ca on $4a$ ($m\bar{3}m$), Te on $4b$ ($m\bar{3}m$), and O on $24e$ ($4m\bar{m}$). Since $\text{Ba}_2\text{CaTeO}_6$ represents the highest possible symmetry of a double perovskite structure (cubic elpasolite-type in space group type $Fm\bar{3}m$), tilting of the $B'\text{O}_6$ or $B''\text{O}_6$ octahedra (Howard *et al.*, 2003), like in the monoclinic structure of $\text{Sr}_2\text{CaTeO}_6$ (Prior *et al.*, 2005), is not observed. The ordering of the CaO_6 and TeO_6 octahedra in a checkerboard arrangement in (III) is displayed in Fig. 2.

With the exception of the Na–O bond length, all other bond lengths (Table 1) are characteristic for their respective coordination polyhedra and in good agreement with mean values compiled recently for alkali and alkaline earth cations bonded to oxygen: K–O = 2.955 Å for coordination number (CN) 9, 3.095 Å for CN 12; Ca–O = 2.668 Å for CN 12; Ba–O = 2.689 Å for CN 6, 2.965 Å for CN 12 (Gagné & Hawthorne, 2016). The same is valid for the mean value of octahedrally coordinated Te^{VI} with a mean Te–O bond length of 1.923 Å (Gagné & Hawthorne, 2018). As noted above, the Na–O bond length deviates from the mean value. At 2.3037 (16) Å it is considerably shorter than the mean of 2.441 Å for CN 6 (Gagné & Hawthorne, 2016). Such a compression has also been reported for other $6H$ - BaTiO_3 -type structures containing sodium. For example, the Na–O distance in $\text{K}_3\text{NaOs}_2\text{O}_9$ has nearly the same value [2.313 (6) Å; Mogare *et al.*, 2012] but is reported to be significantly shorter in $\text{Ba}_3\text{NaRuIrO}_9$ [2.058 (9) Å; Lufaso & zur Loye, 2005b].

3. Synthesis and crystallization

$\text{Ba}[\text{H}_4\text{TeO}_6]$ was prepared according to a literature protocol (Engelbrecht & Sladky, 1965) and its purity checked by X-ray powder diffraction. One gram of dried $\text{Ba}[\text{H}_4\text{TeO}_6]$ was mixed with five grams of a KNO_3/KI mixture (stoichiometric ratio 2:1) for (I) or a $\text{KNO}_3/\text{NaNO}_3$ mixture (stoichiometric ratio

1:1) for (II). The mixtures were placed in platinum crucibles and heated within six h to 773 K, held at that temperature for four days and cooled to room temperature within 12 h. The solidified melts were leached out with water and the remaining solid filtered off, washed with water and ethanol. Colourless single crystals with a hexagonal form for both (I) and (II) were selected from the reaction products. In one case a porcelain crucible was used to reproduce the formation of (I). In this batch, very few colourless crystals of $\text{Ba}_2\text{CaTeO}_6$ (III) had formed as a minor by-product. The porcelain crucible is an adventitious source of calcium that is present in feldspars such as oligoclase used for manufacturing.

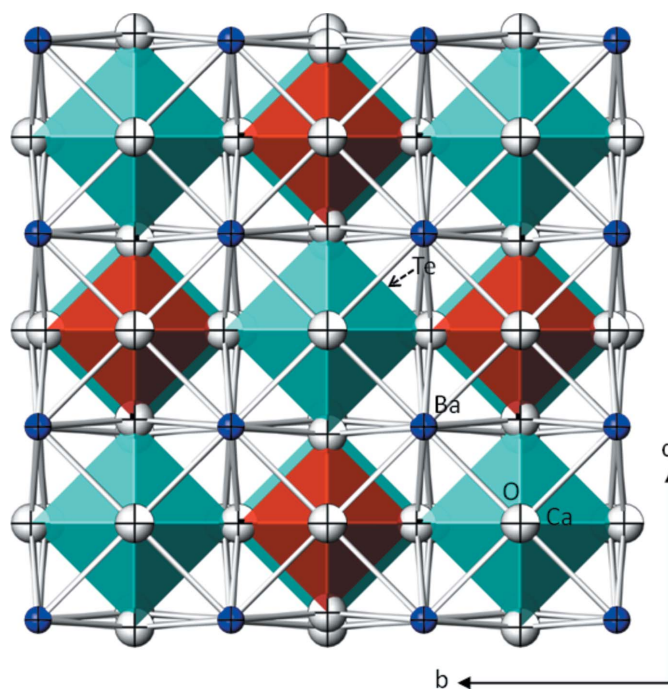


Figure 2
Projection of the crystal structure of $\text{Ba}_2\text{CaTeO}_6$ (III) along $[\bar{1}00]$. $[\text{CaO}_6]$ octahedra are turquoise, $[\text{TeO}_6]$ octahedra are red, Ba sites blue and O sites pale grey. Displacement ellipsoids are drawn at the 97% probability level.

Table 2
Experimental details.

	(I)	(II)	(III)
Crystal data			
Chemical formula	Ba ₂ K ₂ Te ₂ O ₉	Ba ₂ KNaTe ₂ O ₉	Ba ₂ CaTeO ₆
M_r	752.08	735.97	538.36
Crystal system, space group	Hexagonal, $P6_3/mmc$	Hexagonal, $P6_3/mmc$	Cubic, $Fm\bar{3}m$
Temperature (K)	298	293	293
a, b, c (Å)	6.047 (3), 6.047 (3), 16.479 (9)	5.9625 (3), 5.9625 (3), 14.9396 (8)	8.3536 (14), 8.3536 (14), 8.3536 (14)
α, β, γ (°)	90, 90, 120	90, 90, 120	90, 90, 90
V (Å ³)	521.8 (6)	459.97 (5)	582.9 (3)
Z	2	2	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ (mm ⁻¹)	13.80	15.25	19.18
Crystal size (mm)	0.09 × 0.09 × 0.01	0.10 × 0.10 × 0.01	0.08 × 0.08 × 0.08
Data collection			
Diffractometer	Bruker APEXII CCD	Bruker APEXII CCD	Bruker APEXII CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2015)	Multi-scan (SADABS; Bruker, 2015)	Multi-scan (SADABS; Bruker, 2015)
T_{\min} – T_{\max}	0.488, 0.748	0.540, 0.749	0.514, 0.748
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21821, 754, 676	11701, 702, 669	11194, 131, 131
R_{int}	0.041	0.029	0.139
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.943	0.961	0.919
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.015, 0.036, 1.15	0.018, 0.034, 1.49	0.019, 0.049, 1.33
No. of reflections	754	702	131
No. of parameters	22	23	7
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	2.90, -2.02	1.02, -1.63	3.87, -1.68

Computer programs: APEX2 and SAINT (Bruker, 2015), SHELXL2017 (Sheldrick, 2015), ATOMS for Windows (Dowty, 2006) and publCIF (Westrip, 2010).

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. For refinements of (I) and (II) the coordinates of isotypic Ba₃LaRuO₉ (Doi *et al.*, 2002) were used as starting parameters. In the structure of (II), the M1 position with site symmetry $3m$. of Wyckoff site $4f$ is statistically occupied by K⁺ and Ba²⁺ cations. For refinement of (III), the starting parameters were taken from the previous structure determination based on X-ray powder diffraction data (Fu *et al.*, 2008). The type of element on the metal positions was checked by free refinement of the respective site-occupation factors, which confirmed Ca and Ba, respectively.

Funding information

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

References

- Aoba, T., Tiittanen, T., Suematsu, H. & Karppinen, M. (2016). *J. Solid State Chem.* **233**, 492–496.
- Berg, R. W. & Kerridge, D. H. (2004). *Dalton Trans.* pp. 2224–2229.
- Bruker (2015). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Burbank, R. D. & Evans, H. T. (1948). *Acta Cryst.* **1**, 330–336.
- Doi, Y., Matsuhira, K. & Hinatsu, Y. (2002). *J. Solid State Chem.* **165**, 317–323.
- Dowty, E. (2006). *ATOMS for Windows*. Shape Software, 521 Hidden Valley Road, Kingsport, TN 37663, USA.
- Engelbrecht, A. & Sladky, F. (1965). *Monatshfte für Chemie*, **96**, 360–363.
- Fu, W. T., Au, Y. S., Akerboom, S. & Ijdo, D. J. W. (2008). *J. Solid State Chem.* **181**, 2523–2529.
- Gagné, O. C. & Hawthorne, F. C. (2016). *Acta Cryst.* **B72**, 602–625.
- Gagné, O. C. & Hawthorne, F. C. (2018). *Acta Cryst.* **B74**, 63–78.
- Harari, D., Bernier, J. C. & Poix, P. (1972). *J. Solid State Chem.* **5**, 382–390.
- Howard, C. J., Kennedy, B. J. & Woodward, P. M. (2003). *Acta Cryst.* **B59**, 463–471.
- ICSD (2018). The Inorganic Crystal Structure Database. <https://www.fiz-karlsruhe.de/icsd.html>
- Li, M.-R., Deng, Z., Lapidus, S. H., Stephens, P. W., Segre, C. U., Croft, M., Paria Sena, R., Hadermann, J., Walker, D. & Greenblatt, M. (2016). *Inorg. Chem.* **55**, 10135–10142.
- Lufaso, M. W. & zur Loye, H. C. (2005a). *Inorg. Chem.* **44**, 9143–9153.
- Lufaso, M. W. & zur Loye, H. C. (2005b). *Inorg. Chem.* **44**, 9154–9161.
- Mogare, K. M., Klein, W. & Jansen, M. (2012). *J. Solid State Chem.* **191**, 153–157.
- Prior, T. J., Couper, V. J. & Battle, P. D. (2005). *J. Solid State Chem.* **178**, 153–157.
- Sheldrick, G. M. (2015). *Acta Cryst.* **A71**, 3–8.
- Stöger, B., Weil, M. & Zobetz, E. (2010). *Z. Kristallogr.* **225**, 125–138.
- Tilley, R. J. D. (2016). *Perovskites. Structure–Property Relationships*. Chichester: John Wiley & Sons.
- Vasala, S. & Karppinen, M. (2015). *Prog. Solid State Chem.* **43**, 1–36.
- Weil, M. (2016). *Cryst. Growth Des.* **16**, 908–921.
- Weil, M., Stöger, B., Gierl-Mayer, C. & Libowitzky, E. (2016). *J. Solid State Chem.* **241**, 187–197.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
- Zhang, X.-Y., Yao, J.-Y., Jiang, X.-X., Fu, Y., Lin, Z.-H., Zhang, G.-C. & Wu, Y.-C. (2015). *Dalton Trans.* **44**, 15576–15582.

supporting information

Acta Cryst. (2018). E74, 1006-1009 [https://doi.org/10.1107/S2056989018009064]

Crystal structures of the triple perovskites Ba₂K₂Te₂O₉ and Ba₂KNaTe₂O₉, and redetermination of the double perovskite Ba₂CaTeO₆

Matthias Weil

Computing details

For all structures, data collection: *APEX2* (Bruker, 2015); cell refinement: *SAINTE* (Bruker, 2015); data reduction: *SAINTE* (Bruker, 2015). Program(s) used to solve structure: coordinates taken from an isotypic compound for (I), (II); coordinates taken from isotypic compound for (III). Program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015) for (I), (II); *SHELXL2017* (Sheldrick, 2015) for (III). For all structures, molecular graphics: *ATOMS for Windows* (Dowty, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Dibarium dipotassium nonaoxidoditellurate (I)

Crystal data

Ba ₂ K ₂ Te ₂ O ₉	$D_x = 4.786 \text{ Mg m}^{-3}$
$M_r = 752.08$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hexagonal, $P6_3/mmc$	Cell parameters from 9371 reflections
$a = 6.047 (3) \text{ \AA}$	$\theta = 3.9\text{--}42.1^\circ$
$c = 16.479 (9) \text{ \AA}$	$\mu = 13.80 \text{ mm}^{-1}$
$V = 521.8 (6) \text{ \AA}^3$	$T = 298 \text{ K}$
$Z = 2$	Plate, colourless
$F(000) = 652$	$0.09 \times 0.09 \times 0.01 \text{ mm}$

Data collection

Bruker APEXII CCD diffractometer	754 independent reflections
ω - and ϕ -scans	676 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2015)	$R_{\text{int}} = 0.041$
$T_{\text{min}} = 0.488$, $T_{\text{max}} = 0.748$	$\theta_{\text{max}} = 42.1^\circ$, $\theta_{\text{min}} = 3.9^\circ$
21821 measured reflections	$h = -11 \rightarrow 11$
	$k = -11 \rightarrow 11$
	$l = -31 \rightarrow 30$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0151P)^2 + 0.8791P]$
Least-squares matrix: full	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.015$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$wR(F^2) = 0.036$	$\Delta\rho_{\text{max}} = 2.90 \text{ e \AA}^{-3}$
$S = 1.15$	$\Delta\rho_{\text{min}} = -2.02 \text{ e \AA}^{-3}$
754 reflections	Extinction correction: <i>SHELXL2014</i>
22 parameters	(Sheldrick, 2015),
0 restraints	$Fc^* = kFc[1 + 0.001x Fc^2\lambda^3/\sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.0138 (4)

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>	$U_{\text{iso}}^*/U_{\text{eq}}$
K1	0.3333	0.6667	0.87422 (7)	0.02257 (17)
Ba1	0.0000	0.0000	0.2500	0.00960 (5)
Te1	0.3333	0.6667	0.16206 (2)	0.00664 (4)
Ba2	0.0000	0.0000	0.0000	0.00851 (5)
O1	0.47142 (19)	0.9428 (4)	0.2500	0.0117 (3)
O2	0.17636 (16)	0.3527 (3)	0.38974 (10)	0.0198 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.0158 (2)	0.0158 (2)	0.0360 (5)	0.00792 (10)	0.000	0.000
Ba1	0.00959 (6)	0.00959 (6)	0.00961 (9)	0.00480 (3)	0.000	0.000
Te1	0.00661 (5)	0.00661 (5)	0.00671 (7)	0.00330 (3)	0.000	0.000
Ba2	0.00995 (6)	0.00995 (6)	0.00562 (8)	0.00498 (3)	0.000	0.000
O1	0.0150 (6)	0.0068 (7)	0.0106 (7)	0.0034 (3)	0.000	0.000
O2	0.0264 (6)	0.0116 (6)	0.0165 (6)	0.0058 (3)	0.0037 (3)	0.0075 (5)

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

K1—O1 ⁱ	2.893 (2)	Ba1—O1 ^{xvii}	3.0382 (17)
K1—O1 ⁱⁱ	2.893 (2)	Ba1—O1 ^{xviii}	3.0382 (17)
K1—O1 ⁱⁱⁱ	2.893 (2)	Ba1—O1 ^{xix}	3.0382 (17)
K1—O2 ^{iv}	3.0359 (17)	Ba1—O1 ^{xx}	3.0382 (17)
K1—O2 ^v	3.0359 (17)	Te1—O2 ^{xiii}	1.8524 (18)
K1—O2 ^{vi}	3.0359 (17)	Te1—O2 ^{xxi}	1.8524 (18)
K1—O2 ^{vii}	3.0359 (17)	Te1—O2 ^{xxii}	1.8525 (18)
K1—O2 ^{viii}	3.0360 (17)	Te1—O1	2.0474 (16)
K1—O2 ^{ix}	3.0360 (17)	Te1—O1 ^{xvii}	2.0474 (16)
Ba1—O2 ^x	2.952 (2)	Te1—O1 ^{xv}	2.0474 (16)
Ba1—O2 ^{xi}	2.952 (2)	Ba2—O2 ^x	2.5910 (18)
Ba1—O2	2.952 (2)	Ba2—O2 ^{xxiii}	2.5910 (18)
Ba1—O2 ^{xii}	2.952 (2)	Ba2—O2 ^{xiii}	2.5911 (18)
Ba1—O2 ^{xiii}	2.952 (2)	Ba2—O2 ^{xxiv}	2.5911 (18)
Ba1—O2 ^{xiv}	2.952 (2)	Ba2—O2 ^{xii}	2.5911 (18)
Ba1—O1 ^{xv}	3.0382 (17)	Ba2—O2 ^{xxv}	2.5911 (18)
Ba1—O1 ^{xvi}	3.0382 (17)		
O1 ⁱ —K1—O1 ⁱⁱ	75.48 (6)	O1 ^{xvi} —Ba1—O1 ^{xviii}	48.69 (7)
O1 ⁱ —K1—O1 ⁱⁱⁱ	75.48 (6)	O1 ^{xvii} —Ba1—O1 ^{xviii}	71.31 (7)

O1 ⁱⁱ —K1—O1 ⁱⁱⁱ	75.48 (6)	O2 ^x —Ba1—O1 ^{xix}	55.25 (3)
O1 ⁱ —K1—O2 ^{iv}	94.78 (4)	O2 ^{xi} —Ba1—O1 ^{xix}	55.25 (3)
O1 ⁱⁱ —K1—O2 ^{iv}	55.82 (4)	O2—Ba1—O1 ^{xix}	120.56 (3)
O1 ⁱⁱⁱ —K1—O2 ^{iv}	131.10 (5)	O2 ^{xii} —Ba1—O1 ^{xix}	93.53 (2)
O1 ⁱ —K1—O2 ^v	55.82 (4)	O2 ^{xiii} —Ba1—O1 ^{xix}	120.56 (3)
O1 ⁱⁱ —K1—O2 ^v	94.78 (4)	O2 ^{xiv} —Ba1—O1 ^{xix}	93.53 (2)
O1 ⁱⁱⁱ —K1—O2 ^v	131.10 (5)	O1 ^{xv} —Ba1—O1 ^{xix}	120.0
O2 ^{iv} —K1—O2 ^v	63.59 (6)	O1 ^{xvi} —Ba1—O1 ^{xix}	71.31 (8)
O1 ⁱ —K1—O2 ^{vi}	131.10 (5)	O1 ^{xvii} —Ba1—O1 ^{xix}	168.69 (8)
O1 ⁱⁱ —K1—O2 ^{vi}	55.82 (4)	O1 ^{xviii} —Ba1—O1 ^{xix}	120.0
O1 ⁱⁱⁱ —K1—O2 ^{vi}	94.77 (4)	O2 ^x —Ba1—O1 ^{xx}	55.25 (4)
O2 ^{iv} —K1—O2 ^{vi}	55.94 (7)	O2 ^{xi} —Ba1—O1 ^{xx}	55.25 (3)
O2 ^v —K1—O2 ^{vi}	119.299 (12)	O2—Ba1—O1 ^{xx}	93.53 (2)
O1 ⁱ —K1—O2 ^{vii}	55.82 (4)	O2 ^{xii} —Ba1—O1 ^{xx}	120.56 (3)
O1 ⁱⁱ —K1—O2 ^{vii}	131.10 (5)	O2 ^{xiii} —Ba1—O1 ^{xx}	93.53 (2)
O1 ⁱⁱⁱ —K1—O2 ^{vii}	94.78 (4)	O2 ^{xiv} —Ba1—O1 ^{xx}	120.56 (3)
O2 ^{iv} —K1—O2 ^{vii}	119.299 (12)	O1 ^{xv} —Ba1—O1 ^{xx}	71.31 (8)
O2 ^v —K1—O2 ^{vii}	55.94 (7)	O1 ^{xvi} —Ba1—O1 ^{xx}	120.0
O2 ^{vi} —K1—O2 ^{vii}	169.60 (8)	O1 ^{xvii} —Ba1—O1 ^{xx}	120.0
O1 ⁱ —K1—O2 ^{viii}	131.10 (5)	O1 ^{xviii} —Ba1—O1 ^{xx}	168.69 (8)
O1 ⁱⁱ —K1—O2 ^{viii}	94.78 (4)	O1 ^{xix} —Ba1—O1 ^{xx}	48.69 (8)
O1 ⁱⁱⁱ —K1—O2 ^{viii}	55.82 (4)	O2 ^{xiii} —Te1—O2 ^{xxi}	100.46 (7)
O2 ^{iv} —K1—O2 ^{viii}	119.298 (12)	O2 ^{xiii} —Te1—O2 ^{xxii}	100.45 (7)
O2 ^v —K1—O2 ^{viii}	169.60 (8)	O2 ^{xxi} —Te1—O2 ^{xxii}	100.45 (7)
O2 ^{vi} —K1—O2 ^{viii}	63.59 (6)	O2 ^{xiii} —Te1—O1	162.38 (7)
O2 ^{vii} —K1—O2 ^{viii}	119.297 (12)	O2 ^{xxi} —Te1—O1	90.73 (6)
O1 ⁱ —K1—O2 ^{ix}	94.78 (4)	O2 ^{xxii} —Te1—O1	90.73 (6)
O1 ⁱⁱ —K1—O2 ^{ix}	131.10 (5)	O2 ^{xiii} —Te1—O1 ^{xvii}	90.73 (6)
O1 ⁱⁱⁱ —K1—O2 ^{ix}	55.82 (4)	O2 ^{xxi} —Te1—O1 ^{xvii}	162.38 (7)
O2 ^{iv} —K1—O2 ^{ix}	169.60 (8)	O2 ^{xxii} —Te1—O1 ^{xvii}	90.73 (6)
O2 ^v —K1—O2 ^{ix}	119.298 (12)	O1—Te1—O1 ^{xvii}	75.43 (7)
O2 ^{vi} —K1—O2 ^{ix}	119.297 (12)	O2 ^{xiii} —Te1—O1 ^{xv}	90.73 (6)
O2 ^{vii} —K1—O2 ^{ix}	63.59 (6)	O2 ^{xxi} —Te1—O1 ^{xv}	90.73 (6)
O2 ^{viii} —K1—O2 ^{ix}	55.93 (7)	O2 ^{xxii} —Te1—O1 ^{xv}	162.38 (7)
O2 ^x —Ba1—O2 ^{xi}	102.53 (7)	O1—Te1—O1 ^{xv}	75.43 (7)
O2 ^x —Ba1—O2	143.54 (3)	O1 ^{xvii} —Te1—O1 ^{xv}	75.43 (7)
O2 ^{xi} —Ba1—O2	65.62 (6)	O2 ^x —Ba2—O2 ^{xxiii}	180.00 (5)
O2 ^x —Ba1—O2 ^{xii}	65.62 (6)	O2 ^x —Ba2—O2 ^{xiii}	76.25 (7)
O2 ^{xi} —Ba1—O2 ^{xii}	143.54 (3)	O2 ^{xxiii} —Ba2—O2 ^{xiii}	103.75 (7)
O2—Ba1—O2 ^{xii}	143.54 (3)	O2 ^x —Ba2—O2 ^{xxiv}	103.75 (7)
O2 ^x —Ba1—O2 ^{xiii}	65.62 (6)	O2 ^{xxiii} —Ba2—O2 ^{xxiv}	76.25 (7)
O2 ^{xi} —Ba1—O2 ^{xiii}	143.54 (3)	O2 ^{xiii} —Ba2—O2 ^{xxiv}	180.00 (8)
O2—Ba1—O2 ^{xiii}	102.53 (7)	O2 ^x —Ba2—O2 ^{xii}	76.25 (7)
O2 ^{xii} —Ba1—O2 ^{xiii}	65.62 (6)	O2 ^{xxiii} —Ba2—O2 ^{xii}	103.75 (7)
O2 ^x —Ba1—O2 ^{xiv}	143.54 (3)	O2 ^{xiii} —Ba2—O2 ^{xii}	76.25 (7)
O2 ^{xi} —Ba1—O2 ^{xiv}	65.62 (6)	O2 ^{xxiv} —Ba2—O2 ^{xii}	103.75 (7)
O2—Ba1—O2 ^{xiv}	65.62 (6)	O2 ^x —Ba2—O2 ^{xxv}	103.75 (7)
O2 ^{xii} —Ba1—O2 ^{xiv}	102.53 (7)	O2 ^{xxiii} —Ba2—O2 ^{xxv}	76.25 (7)

O2 ^{xiii} —Ba1—O2 ^{xiv}	143.54 (3)	O2 ^{xiii} —Ba2—O2 ^{xxv}	103.75 (7)
O2 ^x —Ba1—O1 ^{xv}	93.53 (2)	O2 ^{xxiv} —Ba2—O2 ^{xxv}	76.25 (7)
O2 ^{xi} —Ba1—O1 ^{xv}	93.53 (2)	O2 ^{xii} —Ba2—O2 ^{xxv}	180.00 (5)
O2—Ba1—O1 ^{xv}	55.25 (3)	Te1 ^{xiii} —O1—Te1	90.11 (9)
O2 ^{xii} —Ba1—O1 ^{xv}	120.56 (3)	Te1 ^{xiii} —O1—K1 ^{xxvi}	89.91 (5)
O2 ^{xiii} —Ba1—O1 ^{xv}	55.25 (4)	Te1—O1—K1 ^{xxvi}	179.97 (5)
O2 ^{xiv} —Ba1—O1 ^{xv}	120.56 (3)	Te1 ^{xiii} —O1—K1 ⁱⁱ	179.97 (12)
O2 ^x —Ba1—O1 ^{xvi}	93.53 (2)	Te1—O1—K1 ⁱⁱ	89.91 (5)
O2 ^{xi} —Ba1—O1 ^{xvi}	93.53 (2)	K1 ^{xxvi} —O1—K1 ⁱⁱ	90.06 (8)
O2—Ba1—O1 ^{xvi}	120.56 (3)	Te1 ^{xiii} —O1—Ba1 ^{xxvii}	93.99 (2)
O2 ^{xii} —Ba1—O1 ^{xvi}	55.25 (3)	Te1—O1—Ba1 ^{xxvii}	93.99 (2)
O2 ^{xiii} —Ba1—O1 ^{xvi}	120.56 (3)	K1 ^{xxvi} —O1—Ba1 ^{xxvii}	86.01 (3)
O2 ^{xiv} —Ba1—O1 ^{xvi}	55.25 (3)	K1 ⁱⁱ —O1—Ba1 ^{xxvii}	86.01 (3)
O1 ^{xv} —Ba1—O1 ^{xvi}	168.69 (7)	Te1 ^{xiii} —O1—Ba1 ^{xxviii}	93.99 (2)
O2 ^x —Ba1—O1 ^{xvii}	120.56 (3)	Te1—O1—Ba1 ^{xxviii}	93.99 (2)
O2 ^{xi} —Ba1—O1 ^{xvii}	120.56 (3)	K1 ^{xxvi} —O1—Ba1 ^{xxviii}	86.01 (3)
O2—Ba1—O1 ^{xvii}	55.25 (3)	K1 ⁱⁱ —O1—Ba1 ^{xxviii}	86.01 (3)
O2 ^{xii} —Ba1—O1 ^{xvii}	93.53 (2)	Ba1 ^{xxvii} —O1—Ba1 ^{xxviii}	168.69 (7)
O2 ^{xiii} —Ba1—O1 ^{xvii}	55.24 (3)	Te1 ^{xiii} —O2—Ba2 ^{xxix}	162.91 (9)
O2 ^{xiv} —Ba1—O1 ^{xvii}	93.53 (2)	Te1 ^{xiii} —O2—Ba1	101.29 (8)
O1 ^{xv} —Ba1—O1 ^{xvii}	48.69 (8)	Ba2 ^{xxix} —O2—Ba1	95.79 (7)
O1 ^{xvi} —Ba1—O1 ^{xviii}	120.0	Te1 ^{xiii} —O2—K1 ^{xxx}	89.48 (3)
O2 ^x —Ba1—O1 ^{xviii}	120.56 (3)	Ba2 ^{xxix} —O2—K1 ^{xxx}	92.02 (3)
O2 ^{xi} —Ba1—O1 ^{xviii}	120.56 (3)	Ba1—O2—K1 ^{xxx}	85.03 (4)
O2—Ba1—O1 ^{xviii}	93.53 (2)	Te1 ^{xiii} —O2—K1 ^{xxxi}	89.48 (3)
O2 ^{xii} —Ba1—O1 ^{xviii}	55.24 (3)	Ba2 ^{xxix} —O2—K1 ^{xxxi}	92.02 (3)
O2 ^{xiii} —Ba1—O1 ^{xviii}	93.53 (2)	Ba1—O2—K1 ^{xxxi}	85.03 (4)
O2 ^{xiv} —Ba1—O1 ^{xviii}	55.24 (3)	K1 ^{xxx} —O2—K1 ^{xxxi}	169.60 (8)
O1 ^{xv} —Ba1—O1 ^{xviii}	120.0		

Symmetry codes: (i) $y-1, -x+y, -z+1$; (ii) $-x+1, -y+2, -z+1$; (iii) $x-y+1, x, -z+1$; (iv) $y, -x+y+1, z+1/2$; (v) $-x, -y+1, z+1/2$; (vi) $x-y+1, x+1, z+1/2$; (vii) $x-y, x, z+1/2$; (viii) $-x+1, -y+1, z+1/2$; (ix) $y, -x+y, z+1/2$; (x) $-x+y, -x, -z+1/2$; (xi) $-x+y, -x, z$; (xii) $-y, x-y, -z+1/2$; (xiii) $x, y, -z+1/2$; (xiv) $-y, x-y, z$; (xv) $-x+y, -x+1, z$; (xvi) $-x+y-1, -x, z$; (xvii) $-y+1, x-y+1, z$; (xviii) $x-1, y-1, z$; (xix) $-y+1, x-y, z$; (xx) $x, y-1, z$; (xxi) $-y+1, x-y+1, -z+1/2$; (xxii) $-x+y, -x+1, -z+1/2$; (xxiii) $x-y, x, z-1/2$; (xxiv) $-x, -y, z-1/2$; (xxv) $y, -x+y, z-1/2$; (xxvi) $-x+1, -y+2, z-1/2$; (xxvii) $x, y+1, z$; (xxviii) $x+1, y+1, z$; (xxix) $-x, -y, z+1/2$; (xxx) $-x+1, -y+1, z-1/2$; (xxxi) $-x, -y+1, z-1/2$.

Dibarium potassium sodium nonaoxidotellurate (II)

Crystal data

Ba₂KNaTe₂O₉

$M_r = 735.97$

Hexagonal, $P6_3/mmc$

$a = 5.9625$ (3) Å

$c = 14.9396$ (8) Å

$V = 459.97$ (5) Å³

$Z = 2$

$F(000) = 636$

$D_x = 5.314$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9985 reflections

$\theta = 2.7\text{--}42.9^\circ$

$\mu = 15.25$ mm⁻¹

$T = 293$ K

Plate, colourless

$0.10 \times 0.10 \times 0.01$ mm

Data collection

Bruker APEXII CCD
diffractometer

ω - and φ -scans

Absorption correction: multi-scan
(SADABS; Bruker, 2015)

$T_{\min} = 0.540$, $T_{\max} = 0.749$

11701 measured reflections

702 independent reflections

669 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 43.1^\circ$, $\theta_{\min} = 2.7^\circ$

$h = -11 \rightarrow 11$

$k = -11 \rightarrow 8$

$l = -28 \rightarrow 28$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.018$

$wR(F^2) = 0.034$

$S = 1.49$

702 reflections

23 parameters

0 restraints

$w = 1/[\sigma^2(F_o^2) + (0.0075P)^2 + 0.5711P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.02 \text{ e } \text{Å}^{-3}$

$\Delta\rho_{\min} = -1.63 \text{ e } \text{Å}^{-3}$

Extinction correction: SHELXL2014

(Sheldrick, 2015),

$F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0409 (10)

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 (Å^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
BaK1	0.3333	0.6667	0.91703 (2)	0.01251 (6)	0.5
KBA1	0.3333	0.6667	0.91703 (2)	0.01251 (6)	0.5
Ba1	0.0000	0.0000	0.2500	0.00953 (5)	
Te1	0.3333	0.6667	0.15383 (2)	0.00583 (5)	
Na2	0.0000	0.0000	0.0000	0.0110 (3)	
O1	0.47381 (18)	0.9476 (4)	0.2500	0.0101 (3)	
O2	0.17638 (16)	0.3528 (3)	0.40559 (12)	0.0195 (3)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
BaK1	0.01060 (8)	0.01060 (8)	0.01631 (11)	0.00530 (4)	0.000	0.000
KBA1	0.01060 (8)	0.01060 (8)	0.01631 (11)	0.00530 (4)	0.000	0.000
Ba1	0.00874 (7)	0.00874 (7)	0.01112 (9)	0.00437 (3)	0.000	0.000
Te1	0.00573 (5)	0.00573 (5)	0.00603 (7)	0.00287 (3)	0.000	0.000
Na2	0.0118 (5)	0.0118 (5)	0.0094 (7)	0.0059 (2)	0.000	0.000
O1	0.0107 (5)	0.0060 (6)	0.0121 (6)	0.0030 (3)	0.000	0.000
O2	0.0235 (6)	0.0120 (6)	0.0192 (6)	0.0060 (3)	0.0045 (3)	0.0089 (5)

Geometric parameters (Å, °)

BaK1—O2 ⁱ	2.9878 (2)	Ba1—O1 ^{xviii}	2.9935 (14)
BaK1—O2 ⁱⁱ	2.9878 (2)	Ba1—O1 ^{xix}	2.9935 (14)
BaK1—O2 ⁱⁱⁱ	2.9878 (2)	Ba1—O1 ^{xx}	2.9935 (14)
BaK1—O2 ^{iv}	2.9878 (2)	Ba1—O1 ^{xxi}	2.9935 (14)
BaK1—O2 ^v	2.9878 (2)	Ba1—O1 ^{xxii}	2.9935 (14)
BaK1—O2 ^{vi}	2.9879 (2)	Ba1—O1 ^{xxiii}	2.9935 (14)
BaK1—O2 ^{vii}	3.1064 (18)	Te1—O2 ^{xxiv}	1.8481 (16)
BaK1—O2 ^{viii}	3.1064 (19)	Te1—O2 ^{xiv}	1.8481 (16)
BaK1—O2 ^{ix}	3.1064 (19)	Te1—O2 ^{xxv}	1.8481 (16)
BaK1—O1 ^x	3.1927 (12)	Te1—O1 ^{xx}	2.0418 (14)
BaK1—O1 ^{xi}	3.1927 (12)	Te1—O1 ^{xviii}	2.0418 (14)
BaK1—O1 ^{xii}	3.1927 (12)	Te1—O1	2.0418 (14)
Ba1—O2 ^{xiii}	2.9532 (18)	Na2—O2 ^{xiv}	2.3037 (16)
Ba1—O2 ^{xiv}	2.9532 (18)	Na2—O2 ^{xxvi}	2.3037 (16)
Ba1—O2 ^{xv}	2.9532 (18)	Na2—O2 ^{xiii}	2.3037 (16)
Ba1—O2	2.9532 (18)	Na2—O2 ^{xxvii}	2.3037 (16)
Ba1—O2 ^{xvi}	2.9532 (18)	Na2—O2 ^{xvi}	2.3038 (16)
Ba1—O2 ^{xvii}	2.9532 (18)	Na2—O2 ^{xxviii}	2.3038 (16)
O2 ⁱ —BaK1—O2 ⁱⁱ	56.05 (6)	O2 ^{xv} —Ba1—O1 ^{xxii}	93.19 (2)
O2 ⁱ —BaK1—O2 ⁱⁱⁱ	63.74 (7)	O2—Ba1—O1 ^{xxii}	120.27 (3)
O2 ⁱⁱ —BaK1—O2 ⁱⁱⁱ	119.677 (7)	O2 ^{xvi} —Ba1—O1 ^{xxii}	55.95 (3)
O2 ⁱ —BaK1—O2 ^{iv}	119.677 (7)	O2 ^{xvii} —Ba1—O1 ^{xxii}	55.95 (3)
O2 ⁱⁱ —BaK1—O2 ^{iv}	63.74 (7)	O1 ^{xviii} —Ba1—O1 ^{xxii}	120.0
O2 ⁱⁱⁱ —BaK1—O2 ^{iv}	172.40 (6)	O1 ^{xix} —Ba1—O1 ^{xxii}	70.37 (7)
O2 ⁱ —BaK1—O2 ^v	119.676 (7)	O1 ^{xx} —Ba1—O1 ^{xxii}	169.63 (7)
O2 ⁱⁱ —BaK1—O2 ^v	172.40 (6)	O1 ^{xxi} —Ba1—O1 ^{xxii}	120.0
O2 ⁱⁱⁱ —BaK1—O2 ^v	56.04 (6)	O2 ^{xxii} —Ba1—O1 ^{xxiii}	120.27 (3)
O2 ^{iv} —BaK1—O2 ^v	119.675 (7)	O2 ^{xiv} —Ba1—O1 ^{xxiii}	93.19 (2)
O2 ⁱ —BaK1—O2 ^{vi}	172.40 (6)	O2 ^{xv} —Ba1—O1 ^{xxiii}	120.27 (3)
O2 ⁱⁱ —BaK1—O2 ^{vi}	119.676 (7)	O2—Ba1—O1 ^{xxiii}	93.20 (2)
O2 ⁱⁱⁱ —BaK1—O2 ^{vi}	119.675 (7)	O2 ^{xvi} —Ba1—O1 ^{xxiii}	55.95 (3)
O2 ^{iv} —BaK1—O2 ^{vi}	56.04 (6)	O2 ^{xvii} —Ba1—O1 ^{xxiii}	55.95 (3)
O2 ^v —BaK1—O2 ^{vi}	63.74 (6)	O1 ^{xviii} —Ba1—O1 ^{xxiii}	70.37 (7)
O2 ⁱ —BaK1—O2 ^{vii}	120.56 (3)	O1 ^{xix} —Ba1—O1 ^{xxiii}	120.0
O2 ⁱⁱ —BaK1—O2 ^{vii}	120.56 (3)	O1 ^{xx} —Ba1—O1 ^{xxiii}	120.0
O2 ⁱⁱⁱ —BaK1—O2 ^{vii}	91.79 (4)	O1 ^{xxi} —Ba1—O1 ^{xxiii}	169.63 (7)
O2 ^{iv} —BaK1—O2 ^{vii}	91.79 (4)	O1 ^{xxii} —Ba1—O1 ^{xxiii}	49.63 (7)
O2 ^v —BaK1—O2 ^{vii}	66.84 (5)	O2 ^{xxiv} —Te1—O2 ^{xiv}	98.85 (7)
O2 ^{vi} —BaK1—O2 ^{vii}	66.84 (5)	O2 ^{xxiv} —Te1—O2 ^{xxv}	98.85 (7)
O2 ⁱ —BaK1—O2 ^{viii}	91.79 (4)	O2 ^{xiv} —Te1—O2 ^{xxv}	98.85 (7)
O2 ⁱⁱ —BaK1—O2 ^{viii}	66.84 (5)	O2 ^{xxiv} —Te1—O1 ^{xx}	91.52 (5)
O2 ⁱⁱⁱ —BaK1—O2 ^{viii}	120.56 (3)	O2 ^{xiv} —Te1—O1 ^{xx}	91.51 (5)
O2 ^{iv} —BaK1—O2 ^{viii}	66.84 (5)	O2 ^{xxv} —Te1—O1 ^{xx}	163.99 (7)
O2 ^v —BaK1—O2 ^{viii}	120.56 (3)	O2 ^{xxiv} —Te1—O1 ^{xviii}	163.99 (7)
O2 ^{vi} —BaK1—O2 ^{viii}	91.79 (4)	O2 ^{xiv} —Te1—O1 ^{xviii}	91.51 (5)

O2 ^{vii} —BaK1—O2 ^{viii}	53.73 (5)	O2 ^{xxv} —Te1—O1 ^{xviii}	91.51 (5)
O2 ⁱ —BaK1—O2 ^{ix}	66.84 (5)	O1 ^{xx} —Te1—O1 ^{xviii}	75.95 (6)
O2 ⁱⁱ —BaK1—O2 ^{ix}	91.79 (4)	O2 ^{xxiv} —Te1—O1	91.51 (5)
O2 ⁱⁱⁱ —BaK1—O2 ^{ix}	66.84 (5)	O2 ^{xiv} —Te1—O1	163.99 (7)
O2 ^{iv} —BaK1—O2 ^{ix}	120.56 (3)	O2 ^{xxv} —Te1—O1	91.52 (5)
O2 ^v —BaK1—O2 ^{ix}	91.79 (4)	O1 ^{xx} —Te1—O1	75.95 (6)
O2 ^{vi} —BaK1—O2 ^{ix}	120.56 (3)	O1 ^{xviii} —Te1—O1	75.95 (6)
O2 ^{vii} —BaK1—O2 ^{ix}	53.73 (5)	O2 ^{xiv} —Na2—O2 ^{xxvi}	180.00 (9)
O2 ^{viii} —BaK1—O2 ^{ix}	53.73 (5)	O2 ^{xiv} —Na2—O2 ^{xiii}	86.43 (7)
O2 ⁱ —BaK1—O1 ^x	88.64 (4)	O2 ^{xxvi} —Na2—O2 ^{xiii}	93.57 (7)
O2 ⁱⁱ —BaK1—O1 ^x	118.94 (4)	O2 ^{xiv} —Na2—O2 ^{xxvii}	93.57 (7)
O2 ⁱⁱⁱ —BaK1—O1 ^x	53.54 (4)	O2 ^{xxvi} —Na2—O2 ^{xxvii}	86.43 (7)
O2 ^{iv} —BaK1—O1 ^x	118.94 (4)	O2 ^{xiii} —Na2—O2 ^{xxvii}	180.00 (9)
O2 ^v —BaK1—O1 ^x	53.54 (4)	O2 ^{xiv} —Na2—O2 ^{xvi}	86.43 (7)
O2 ^{vi} —BaK1—O1 ^x	88.64 (4)	O2 ^{xxvi} —Na2—O2 ^{xvi}	93.57 (7)
O2 ^{vii} —BaK1—O1 ^x	120.26 (3)	O2 ^{xiii} —Na2—O2 ^{xvi}	86.43 (7)
O2 ^{viii} —BaK1—O1 ^x	172.86 (4)	O2 ^{xxvii} —Na2—O2 ^{xvi}	93.57 (7)
O2 ^{ix} —BaK1—O1 ^x	120.26 (3)	O2 ^{xiv} —Na2—O2 ^{xxviii}	93.57 (7)
O2 ⁱ —BaK1—O1 ^{xi}	118.94 (4)	O2 ^{xxvi} —Na2—O2 ^{xxviii}	86.43 (7)
O2 ⁱⁱ —BaK1—O1 ^{xi}	88.64 (4)	O2 ^{xiii} —Na2—O2 ^{xxviii}	93.57 (7)
O2 ⁱⁱⁱ —BaK1—O1 ^{xi}	118.94 (4)	O2 ^{xxvii} —Na2—O2 ^{xxviii}	86.43 (7)
O2 ^{iv} —BaK1—O1 ^{xi}	53.54 (4)	O2 ^{xvi} —Na2—O2 ^{xxviii}	180.00 (7)
O2 ^v —BaK1—O1 ^{xi}	88.64 (4)	Te1 ^{xiv} —O1—Te1	89.44 (8)
O2 ^{vi} —BaK1—O1 ^{xi}	53.54 (4)	Te1 ^{xiv} —O1—Ba1 ^{xxix}	93.68 (2)
O2 ^{vii} —BaK1—O1 ^{xi}	120.26 (3)	Te1—O1—Ba1 ^{xxix}	93.68 (2)
O2 ^{viii} —BaK1—O1 ^{xi}	120.26 (3)	Te1 ^{xiv} —O1—Ba1 ^{xxx}	93.68 (2)
O2 ^{ix} —BaK1—O1 ^{xi}	172.86 (4)	Te1—O1—Ba1 ^{xxx}	93.68 (2)
O1 ^x —BaK1—O1 ^{xi}	65.40 (4)	Ba1 ^{xxix} —O1—Ba1 ^{xxx}	169.63 (7)
O2 ⁱ —BaK1—O1 ^{xii}	53.54 (4)	Te1 ^{xiv} —O1—BaK1 ^{xxxi}	83.874 (13)
O2 ⁱⁱ —BaK1—O1 ^{xii}	53.54 (4)	Te1—O1—BaK1 ^{xxxi}	173.32 (6)
O2 ⁱⁱⁱ —BaK1—O1 ^{xii}	88.64 (4)	Ba1 ^{xxix} —O1—BaK1 ^{xxxi}	86.77 (2)
O2 ^{iv} —BaK1—O1 ^{xii}	88.64 (4)	Ba1 ^{xxx} —O1—BaK1 ^{xxxi}	86.77 (2)
O2 ^v —BaK1—O1 ^{xii}	118.94 (4)	Te1 ^{xiv} —O1—KBA1 ^{xxxi}	83.874 (13)
O2 ^{vi} —BaK1—O1 ^{xii}	118.94 (4)	Te1—O1—KBA1 ^{xxxi}	173.32 (6)
O2 ^{vii} —BaK1—O1 ^{xii}	172.86 (4)	Ba1 ^{xxix} —O1—KBA1 ^{xxxi}	86.77 (2)
O2 ^{viii} —BaK1—O1 ^{xii}	120.26 (3)	Ba1 ^{xxx} —O1—KBA1 ^{xxxi}	86.77 (2)
O2 ^{ix} —BaK1—O1 ^{xii}	120.26 (3)	BaK1 ^{xxxi} —O1—KBA1 ^{xxxi}	0.000 (7)
O1 ^x —BaK1—O1 ^{xii}	65.40 (4)	Te1 ^{xiv} —O1—BaK1 ^{xi}	173.32 (6)
O1 ^{xi} —BaK1—O1 ^{xii}	65.40 (4)	Te1—O1—BaK1 ^{xi}	83.874 (13)
O2 ^{xiii} —Ba1—O2 ^{xiv}	64.58 (5)	Ba1 ^{xxix} —O1—BaK1 ^{xi}	86.77 (2)
O2 ^{xiii} —Ba1—O2 ^{xv}	103.83 (6)	Ba1 ^{xxx} —O1—BaK1 ^{xi}	86.77 (2)
O2 ^{xiv} —Ba1—O2 ^{xv}	144.07 (2)	BaK1 ^{xxxi} —O1—BaK1 ^{xi}	102.81 (5)
O2 ^{xiii} —Ba1—O2	144.07 (3)	KBA1 ^{xxxi} —O1—BaK1 ^{xi}	102.8
O2 ^{xiv} —Ba1—O2	103.83 (6)	Te1 ^{xiv} —O1—KBA1 ^{xi}	173.32 (6)
O2 ^{xv} —Ba1—O2	64.58 (5)	Te1—O1—KBA1 ^{xi}	83.874 (13)
O2 ^{xiii} —Ba1—O2 ^{xvi}	64.58 (5)	Ba1 ^{xxix} —O1—KBA1 ^{xi}	86.77 (2)
O2 ^{xiv} —Ba1—O2 ^{xvi}	64.58 (5)	Ba1 ^{xxx} —O1—KBA1 ^{xi}	86.77 (2)
O2 ^{xv} —Ba1—O2 ^{xvi}	144.07 (2)	BaK1 ^{xxxi} —O1—KBA1 ^{xi}	102.81 (5)

O2—Ba1—O2 ^{xvi}	144.07 (2)	KBA1 ^{xxxii} —O1—KBA1 ^{xi}	102.81 (5)
O2 ^{xiii} —Ba1—O2 ^{xvii}	144.07 (3)	BaK1 ^{xi} —O1—KBA1 ^{xi}	0.000 (7)
O2 ^{xiv} —Ba1—O2 ^{xvii}	144.07 (3)	Te1 ^{xiv} —O2—Na2 ^{xxxii}	170.96 (10)
O2 ^{xv} —Ba1—O2 ^{xvii}	64.58 (5)	Te1 ^{xiv} —O2—Ba1	99.37 (7)
O2—Ba1—O2 ^{xvii}	64.58 (5)	Na2 ^{xxxii} —O2—Ba1	89.67 (6)
O2 ^{xvi} —Ba1—O2 ^{xvii}	103.83 (6)	Te1 ^{xiv} —O2—BaK1 ^{xxxiii}	93.26 (3)
O2 ^{xiii} —Ba1—O1 ^{xviii}	120.27 (3)	Na2 ^{xxxii} —O2—BaK1 ^{xxxiii}	86.47 (3)
O2 ^{xiv} —Ba1—O1 ^{xviii}	55.95 (3)	Ba1—O2—BaK1 ^{xxxiii}	91.39 (4)
O2 ^{xv} —Ba1—O1 ^{xviii}	120.27 (3)	Te1 ^{xiv} —O2—KBA1 ^{xxxiii}	93.26 (3)
O2—Ba1—O1 ^{xviii}	55.95 (3)	Na2 ^{xxxii} —O2—KBA1 ^{xxxiii}	86.47 (3)
O2 ^{xvi} —Ba1—O1 ^{xviii}	93.20 (2)	Ba1—O2—KBA1 ^{xxxiii}	91.39 (4)
O2 ^{xvii} —Ba1—O1 ^{xviii}	93.19 (2)	BaK1 ^{xxxiii} —O2—KBA1 ^{xxxiii}	0.000 (13)
O2 ^{xiii} —Ba1—O1 ^{xix}	55.95 (3)	Te1 ^{xiv} —O2—BaK1 ^{xxxiv}	93.26 (3)
O2 ^{xiv} —Ba1—O1 ^{xix}	120.27 (3)	Na2 ^{xxxii} —O2—BaK1 ^{xxxiv}	86.47 (3)
O2 ^{xv} —Ba1—O1 ^{xix}	55.95 (3)	Ba1—O2—BaK1 ^{xxxiv}	91.39 (4)
O2—Ba1—O1 ^{xix}	120.27 (3)	BaK1 ^{xxxiii} —O2—BaK1 ^{xxxiv}	172.40 (6)
O2 ^{xvi} —Ba1—O1 ^{xix}	93.20 (2)	KBA1 ^{xxxiii} —O2—BaK1 ^{xxxiv}	172.4
O2 ^{xvii} —Ba1—O1 ^{xix}	93.20 (2)	Te1 ^{xiv} —O2—KBA1 ^{xxxiv}	93.26 (3)
O1 ^{xviii} —Ba1—O1 ^{xix}	169.63 (7)	Na2 ^{xxxii} —O2—KBA1 ^{xxxiv}	86.47 (3)
O2 ^{xiii} —Ba1—O1 ^{xx}	93.20 (2)	Ba1—O2—KBA1 ^{xxxiv}	91.39 (4)
O2 ^{xiv} —Ba1—O1 ^{xx}	55.95 (3)	BaK1 ^{xxxiii} —O2—KBA1 ^{xxxiv}	172.40 (6)
O2 ^{xv} —Ba1—O1 ^{xx}	93.20 (2)	KBA1 ^{xxxiii} —O2—KBA1 ^{xxxiv}	172.40 (6)
O2—Ba1—O1 ^{xx}	55.95 (3)	BaK1 ^{xxxiv} —O2—KBA1 ^{xxxiv}	0.0
O2 ^{xvi} —Ba1—O1 ^{xx}	120.27 (3)	Te1 ^{xiv} —O2—KBA1 ^{ix}	87.26 (6)
O2 ^{xvii} —Ba1—O1 ^{xx}	120.27 (3)	Na2 ^{xxxii} —O2—KBA1 ^{ix}	83.70 (5)
O1 ^{xviii} —Ba1—O1 ^{xx}	49.63 (7)	Ba1—O2—KBA1 ^{ix}	173.37 (6)
O1 ^{xix} —Ba1—O1 ^{xx}	120.0	BaK1 ^{xxxiii} —O2—KBA1 ^{ix}	88.21 (4)
O2 ^{xiii} —Ba1—O1 ^{xxi}	55.95 (3)	KBA1 ^{xxxiii} —O2—KBA1 ^{ix}	88.21 (4)
O2 ^{xiv} —Ba1—O1 ^{xxi}	93.20 (2)	BaK1 ^{xxxiv} —O2—KBA1 ^{ix}	88.21 (4)
O2 ^{xv} —Ba1—O1 ^{xxi}	55.95 (3)	KBA1 ^{xxxiv} —O2—KBA1 ^{ix}	88.21 (4)
O2—Ba1—O1 ^{xxi}	93.20 (2)	Te1 ^{xiv} —O2—BaK1 ^{ix}	87.26 (6)
O2 ^{xvi} —Ba1—O1 ^{xxi}	120.27 (3)	Na2 ^{xxxii} —O2—BaK1 ^{ix}	83.70 (5)
O2 ^{xvii} —Ba1—O1 ^{xxi}	120.27 (3)	Ba1—O2—BaK1 ^{ix}	173.37 (6)
O1 ^{xviii} —Ba1—O1 ^{xxi}	120.0	BaK1 ^{xxxiii} —O2—BaK1 ^{ix}	88.21 (4)
O1 ^{xix} —Ba1—O1 ^{xxi}	49.63 (7)	KBA1 ^{xxxiii} —O2—BaK1 ^{ix}	88.2
O1 ^{xx} —Ba1—O1 ^{xxi}	70.37 (7)	BaK1 ^{xxxiv} —O2—BaK1 ^{ix}	88.21 (4)
O2 ^{xiii} —Ba1—O1 ^{xxii}	93.19 (2)	KBA1 ^{xxxiv} —O2—BaK1 ^{ix}	88.2
O2 ^{xiv} —Ba1—O1 ^{xxii}	120.27 (3)	KBA1 ^{ix} —O2—BaK1 ^{ix}	0.0

Symmetry codes: (i) $y, -x+y, z+1/2$; (ii) $-x+1, -y+1, z+1/2$; (iii) $x-y, x, z+1/2$; (iv) $x-y+1, x+1, z+1/2$; (v) $-x, -y+1, z+1/2$; (vi) $y, -x+y+1, z+1/2$; (vii) $-x+y, -x+1, -z+3/2$; (viii) $-y+1, x-y+1, -z+3/2$; (ix) $x, y, -z+3/2$; (x) $y-1, -x+y, -z+1$; (xi) $-x+1, -y+2, -z+1$; (xii) $x-y+1, x, -z+1$; (xiii) $-y, x-y, -z+1/2$; (xiv) $x, y, -z+1/2$; (xv) $-y, x-y, z$; (xvi) $-x+y, -x, -z+1/2$; (xvii) $-x+y, -x, z$; (xviii) $-x+y, -x+1, z$; (xix) $-x+y-1, -x, z$; (xx) $-y+1, x-y+1, z$; (xxi) $x-1, y-1, z$; (xxii) $-y+1, x-y, z$; (xxiii) $x, y-1, z$; (xxiv) $-x+y, -x+1, -z+1/2$; (xxv) $-y+1, x-y+1, -z+1/2$; (xxvi) $-x, -y, z-1/2$; (xxvii) $y, -x+y, z-1/2$; (xxviii) $x-y, x, z-1/2$; (xxix) $x+1, y+1, z$; (xxx) $x, y+1, z$; (xxxi) $-x+1, -y+2, z-1/2$; (xxxii) $-x, -y, z+1/2$; (xxxiii) $-x+1, -y+1, z-1/2$; (xxxiv) $-x, -y+1, z-1/2$.

Dibarium calcium hexaoxidotellurate (III)

Crystal data

Ba₂CaTeO₆
M_r = 538.36

Cubic, $Fm\bar{3}m$
a = 8.3536 (14) Å

$V = 582.9 (3) \text{ \AA}^3$
 $Z = 4$
 $F(000) = 928$
 $D_x = 6.134 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 5256 reflections

$\theta = 4.2\text{--}40.4^\circ$
 $\mu = 19.18 \text{ mm}^{-1}$
 $T = 293 \text{ K}$
 Octahedron, colourless
 $0.08 \times 0.08 \times 0.08 \text{ mm}$

Data collection

Bruker APEXII CCD
 diffractometer
 φ - and ω -scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2015)
 $T_{\min} = 0.514$, $T_{\max} = 0.748$
 11194 measured reflections

131 independent reflections
 131 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.139$
 $\theta_{\max} = 40.8^\circ$, $\theta_{\min} = 4.2^\circ$
 $h = -15 \rightarrow 15$
 $k = -15 \rightarrow 15$
 $l = -15 \rightarrow 15$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.019$
 $wR(F^2) = 0.049$
 $S = 1.33$
 131 reflections
 7 parameters

0 restraints
 $w = 1/[\sigma^2(F_o^2) + (0.0237P)^2 + 1.8403P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 3.87 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -1.68 \text{ e \AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ba	0.250000	0.250000	0.250000	0.00957 (13)
Ca	0.000000	0.000000	0.000000	0.0066 (2)
Te	0.500000	0.500000	0.500000	0.00602 (13)
O	0.2690 (4)	0.000000	0.000000	0.0203 (6)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba	0.00957 (13)	0.00957 (13)	0.00957 (13)	0.000	0.000	0.000
Ca	0.0066 (2)	0.0066 (2)	0.0066 (2)	0.000	0.000	0.000
Te	0.00602 (13)	0.00602 (13)	0.00602 (13)	0.000	0.000	0.000
O	0.0201 (12)	0.0203 (8)	0.0203 (8)	0.000	0.000	0.000

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

Ba—O ⁱ	2.9577 (5)	Ca—O	2.247 (3)
Ba—O ⁱⁱ	2.9577 (5)	Ca—O ^{xii}	2.247 (3)
Ba—O	2.9577 (5)	Ca—O ^{iv}	2.247 (3)

Ba—O ⁱⁱⁱ	2.9577 (5)	Ca—O ^{xiii}	2.247 (3)
Ba—O ^{iv}	2.9577 (5)	Ca—O ^v	2.247 (3)
Ba—O ^v	2.9577 (5)	Ca—O ^{xiv}	2.247 (3)
Ba—O ^{vi}	2.9577 (5)	Te—O ^{xv}	1.930 (3)
Ba—O ^{vii}	2.9577 (5)	Te—O ⁱⁱⁱ	1.930 (3)
Ba—O ^{viii}	2.9577 (5)	Te—O ^{xvi}	1.930 (3)
Ba—O ^{ix}	2.9577 (5)	Te—O ⁱ	1.930 (3)
Ba—O ^x	2.9577 (5)	Te—O ^{xvii}	1.930 (3)
Ba—O ^{xi}	2.9577 (5)	Te—O ⁱⁱ	1.930 (3)
O ⁱ —Ba—O ⁱⁱ	54.95 (11)	O ⁱⁱ —Ba—O ^{xi}	90.165 (7)
O ⁱ —Ba—O	119.905 (4)	O—Ba—O ^{xi}	90.165 (7)
O ⁱⁱ —Ba—O	173.85 (13)	O ⁱⁱⁱ —Ba—O ^{xi}	119.905 (4)
O ⁱ —Ba—O ⁱⁱⁱ	54.95 (11)	O ^{iv} —Ba—O ^{xi}	54.95 (11)
O ⁱⁱ —Ba—O ⁱⁱⁱ	54.95 (11)	O ^v —Ba—O ^{xi}	119.905 (4)
O—Ba—O ⁱⁱⁱ	119.905 (4)	O ^{vi} —Ba—O ^{xi}	64.99 (11)
O ⁱ —Ba—O ^{iv}	119.905 (4)	O ^{vii} —Ba—O ^{xi}	119.905 (4)
O ⁱⁱ —Ba—O ^{iv}	119.905 (4)	O ^{viii} —Ba—O ^{xi}	119.905 (4)
O—Ba—O ^{iv}	64.99 (11)	O ^{ix} —Ba—O ^{xi}	54.95 (11)
O ⁱⁱⁱ —Ba—O ^{iv}	173.85 (13)	O ^x —Ba—O ^{xi}	173.85 (13)
O ⁱ —Ba—O ^v	173.85 (13)	O—Ca—O ^{xii}	90.0
O ⁱⁱ —Ba—O ^v	119.905 (4)	O—Ca—O ^{iv}	90.0
O—Ba—O ^v	64.99 (11)	O ^{xii} —Ca—O ^{iv}	180.0
O ⁱⁱⁱ —Ba—O ^v	119.905 (4)	O—Ca—O ^{xiii}	90.0
O ^{iv} —Ba—O ^v	64.99 (11)	O ^{xii} —Ca—O ^{xiii}	90.0
O ⁱ —Ba—O ^{vi}	64.99 (11)	O ^{iv} —Ca—O ^{xiii}	90.0
O ⁱⁱ —Ba—O ^{vi}	119.905 (4)	O—Ca—O ^v	90.0
O—Ba—O ^{vi}	54.95 (11)	O ^{xii} —Ca—O ^v	90.0
O ⁱⁱⁱ —Ba—O ^{vi}	90.165 (7)	O ^{iv} —Ca—O ^v	90.0
O ^{iv} —Ba—O ^{vi}	90.165 (7)	O ^{xiii} —Ca—O ^v	180.0
O ^v —Ba—O ^{vi}	119.905 (4)	O—Ca—O ^{xiv}	180.0
O ⁱ —Ba—O ^{vii}	119.905 (4)	O ^{xii} —Ca—O ^{xiv}	90.0
O ⁱⁱ —Ba—O ^{vii}	64.99 (11)	O ^{iv} —Ca—O ^{xiv}	90.0
O—Ba—O ^{vii}	119.905 (4)	O ^{xiii} —Ca—O ^{xiv}	90.0
O ⁱⁱⁱ —Ba—O ^{vii}	90.165 (7)	O ^v —Ca—O ^{xiv}	90.0
O ^{iv} —Ba—O ^{vii}	90.165 (7)	O ^{xv} —Te—O ⁱⁱⁱ	180.0
O ^v —Ba—O ^{vii}	54.95 (11)	O ^{xv} —Te—O ^{xvi}	90.0
O ^{vi} —Ba—O ^{vii}	173.85 (13)	O ⁱⁱⁱ —Te—O ^{xvi}	90.0
O ⁱ —Ba—O ^{viii}	90.165 (7)	O ^{xv} —Te—O ⁱ	90.0
O ⁱⁱ —Ba—O ^{viii}	119.905 (4)	O ⁱⁱⁱ —Te—O ⁱ	90.0
O—Ba—O ^{viii}	54.95 (11)	O ^{xvi} —Te—O ⁱ	180.0
O ⁱⁱⁱ —Ba—O ^{viii}	64.99 (11)	O ^{xv} —Te—O ^{xvii}	90.000 (1)
O ^{iv} —Ba—O ^{viii}	119.905 (4)	O ⁱⁱⁱ —Te—O ^{xvii}	90.0
O ^v —Ba—O ^{viii}	90.165 (7)	O ^{xvi} —Te—O ^{xvii}	90.000 (1)
O ^{vi} —Ba—O ^{viii}	54.95 (11)	O ⁱ —Te—O ^{xvii}	90.0
O ^{vii} —Ba—O ^{viii}	119.905 (4)	O ^{xv} —Te—O ⁱⁱ	90.0
O ⁱ —Ba—O ^{ix}	90.165 (7)	O ⁱⁱⁱ —Te—O ⁱⁱ	90.000 (1)
O ⁱⁱ —Ba—O ^{ix}	64.99 (11)	O ^{xvi} —Te—O ⁱⁱ	90.0

O—Ba—O ^{ix}	119.905 (4)	O ⁱ —Te—O ⁱⁱ	90.000 (1)
O ⁱⁱⁱ —Ba—O ^{ix}	119.905 (4)	O ^{xvii} —Te—O ⁱⁱ	180.0
O ^{iv} —Ba—O ^{ix}	54.95 (11)	Te ^{xviii} —O—Ca	180.0
O ^v —Ba—O ^{ix}	90.165 (7)	Te ^{xviii} —O—Ba ^{xviii}	93.08 (7)
O ^{vi} —Ba—O ^{ix}	119.905 (4)	Ca—O—Ba ^{xviii}	86.92 (7)
O ^{vii} —Ba—O ^{ix}	64.99 (11)	Te ^{xviii} —O—Ba	93.08 (7)
O ^{viii} —Ba—O ^{ix}	173.85 (13)	Ca—O—Ba	86.92 (7)
O ⁱ —Ba—O ^x	119.905 (4)	Ba ^{xviii} —O—Ba	173.85 (13)
O ⁱⁱ —Ba—O ^x	90.165 (7)	Te ^{xviii} —O—Ba ^x	93.08 (7)
O—Ba—O ^x	90.165 (7)	Ca—O—Ba ^x	86.92 (7)
O ⁱⁱⁱ —Ba—O ^x	64.99 (11)	Ba ^{xviii} —O—Ba ^x	89.835 (7)
O ^{iv} —Ba—O ^x	119.905 (4)	Ba—O—Ba ^x	89.835 (7)
O ^v —Ba—O ^x	54.95 (11)	Te ^{xviii} —O—Ba ^{xi}	93.08 (7)
O ^{vi} —Ba—O ^x	119.905 (4)	Ca—O—Ba ^{xi}	86.92 (7)
O ^{vii} —Ba—O ^x	54.95 (11)	Ba ^{xviii} —O—Ba ^{xi}	89.835 (7)
O ^{viii} —Ba—O ^x	64.99 (11)	Ba—O—Ba ^{xi}	89.835 (7)
O ^{ix} —Ba—O ^x	119.905 (4)	Ba ^x —O—Ba ^{xi}	173.85 (13)
O ⁱ —Ba—O ^{xi}	64.99 (11)		

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