

Crystal structure of dilead(II) oxochromate(VI) oxotellurate(IV)

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Reaction of chromium(III) precursors with TeO_2 in PbF_2/PbO melts in air led to oxidation of chromium(III) to chromium(VI), whereas tellurium remained its oxidation state of IV. In the resulting title compound, $\text{Pb}_2(\text{CrO}_4)(\text{TeO}_3)$, the two types of anions are isolated from each other, hence a double salt is formed. The two independent Pb^{2+} cations exhibit coordination number nine under formation of very distorted coordination polyhedra [bond-length range = 2.363 (6)–3.276 (7) Å]. The oxochromate(VI) and oxotellurate(IV) anions have tetrahedral and trigonal–pyramidal configurations, respectively. In the crystal structure, (001) layers of metal cations alternate with layers of TeO_3^{2-} and CrO_4^{2-} anions along [001], forming a three-dimensional framework structure. $\text{Pb}_2(\text{CrO}_4)(\text{TeO}_3)$ is isotypic with its sulfate analogue $\text{Pb}_2(\text{SO}_4)(\text{TeO}_3)$ and is comparatively discussed.

1. Chemical context

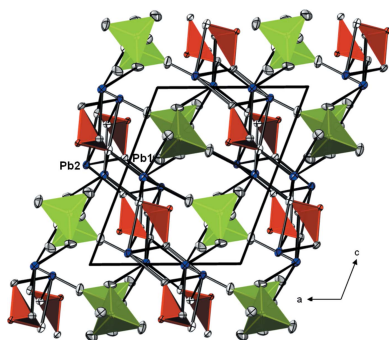
$\text{Pb}_3\text{Fe}_2\text{Te}_2\text{O}_{12}$ is an oxotellurate(VI) with interesting structural features. It crystallizes in the non-centrosymmetric space group Cc and has Te^{VI} and Fe^{III} atoms occupationally disordered at the same sites (Müller-Buschbaum & Wedel, 1997). This compound has been prepared by solid-state reactions from a PbO , Fe_2O_3 and TeO_2 mixture in air, which led to oxidation of Te^{IV} to Te^{VI} . During an attempt to replace iron(III) by chromium(III) to prepare a possible phase with composition ' $\text{Pb}_3\text{Cr}_2\text{Te}_2\text{O}_{12}$ ', the title compound, $\text{Pb}_2(\text{CrO}_4)(\text{TeO}_3)$, was obtained instead while working under similar conditions. Interestingly, chromium was then oxidized ($\text{Cr}^{\text{III}} \rightarrow \text{Cr}^{\text{VI}}$) while tellurium remained its oxidation state of IV. $\text{Pb}_2(\text{CrO}_4)(\text{TeO}_3)$ is isotypic with its sulfate analogue $\text{Pb}_2(\text{SO}_4)(\text{TeO}_3)$ (Weil & Shir Khanlou, 2017).

2. Structural commentary

All atoms in the asymmetric unit, *viz.* two Pb, one Cr, one Te and seven O sites, are located on general positions.

The coordination environments of the two Pb^{2+} cations are markedly different. If only Pb–O bond lengths < 2.8 Å are considered, atom Pb1 is surrounded by six O atoms in the range 2.4–2.8 Å whereas atom Pb2 has four oxygen atoms as coordination partners, three at ~2.38 Å and one at 2.75 Å. Taking into account the more remote oxygen atoms as well, the coordination numbers are increased to nine for both Pb^{2+} cations (Fig. 1, Table 1).

The chromium atom shows a tetrahedral and the tellurium a trigonal–pyramidal coordination by oxygen atoms. These two coordination polyhedra and the corresponding bond lengths



ranges are typical for oxochromates(VI) (Pressprich *et al.*, 1988) and oxotellurates(IV) (Christy *et al.*, 2016), respectively.

In the crystal structure, the Pb^{2+} cations are arranged in layers parallel to (001) at $z \sim 0, \frac{1}{2}$ and in turn are stacked into columns extending along [010]. The two types of anion polyhedra are isolated and are likewise arranged into columnar arrangements along [010], forming anion layers situated at $z \sim \frac{1}{4}$ and $\frac{3}{4}$. The metal cation and anion layers alternate along [001] and build up the three-dimensional framework of the crystal structure. The $5s^2$ and $6s^2$ electron lone pairs of the Te^{IV} atoms of the oxotellurate anions and of the Pb^{2+} cations, respectively, are stereochemically active and point into channels running parallel to the two types of columns along [010] (Fig. 2).

Relevant bond lengths of isotypic $\text{Pb}_2(\text{CrO}_4)(\text{TeO}_3)$ and $\text{Pb}_2(\text{SO}_4)(\text{TeO}_3)$ are compared in Table 1. Whereas the TeO_3^{2-} anions in the two structures show only marginal differences, the expected differences in the $X\text{—O}$ bond lengths ($X = \text{Cr}, \text{S}$) of the chromate and sulfate tetrahedra (average values 1.65 and 1.48 Å, respectively) also have

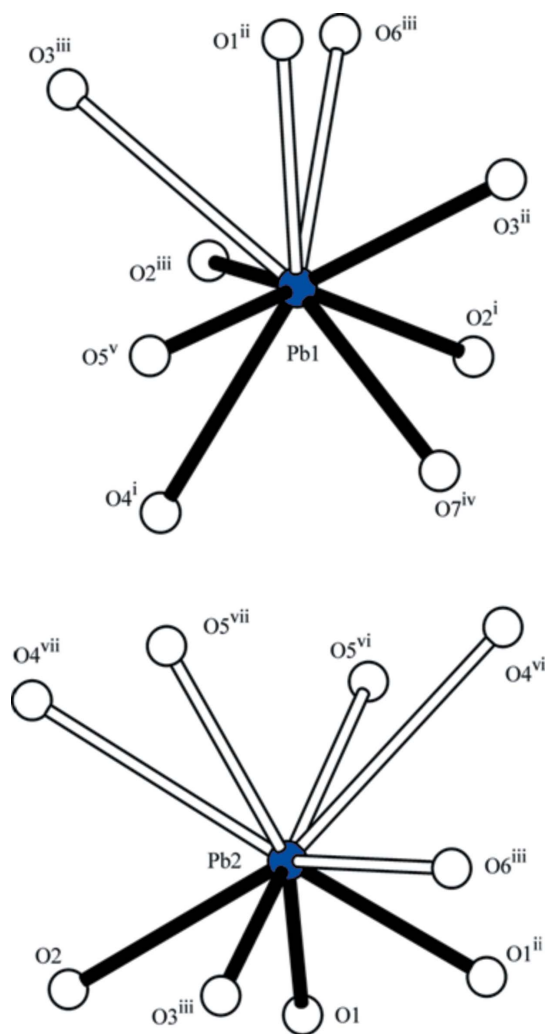


Figure 1
Coordination environments around the two Pb^{2+} cations in $\text{Pb}_2(\text{CrO}_4)(\text{TeO}_3)$. Pb—O bonds < 2.8 Å are given in full and longer Pb—O bonds are open. Symmetry operators refer to Table 1.

Table 1
Comparison of bond lengths between isotypic $\text{Pb}_2(\text{CrO}_4)(\text{TeO}_3)$ and $\text{Pb}_2(\text{SO}_4)(\text{TeO}_3)$.

Bond	$\text{Pb}_2(\text{CrO}_4)(\text{TeO}_3)$	$\text{Pb}_2(\text{SO}_4)(\text{TeO}_3)$
Pb1—O2^{i}	2.429 (6)	2.397 (3)
$\text{Pb1—O3}^{\text{ii}}$	2.573 (6)	2.594 (3)
$\text{Pb1—O2}^{\text{iii}}$	2.594 (6)	2.536 (3)
$\text{Pb1—O7}^{\text{iv}}$	2.617 (7)	2.632 (3)
Pb1—O5^{v}	2.750 (7)	2.789 (3)
Pb1—O4^{i}	2.777 (7)	2.677 (3)
$\text{Pb1—O6}^{\text{iii}}$	2.850 (7)	3.107 (4)
$\text{Pb1—O1}^{\text{ii}}$	2.968 (6)	2.993 (3)
$\text{Pb1—O3}^{\text{iii}}$	3.170 (6)	3.206 (3)
$\text{Pb2—O3}^{\text{iii}}$	2.363 (6)	2.335 (3)
$\text{Pb2—O1}^{\text{ii}}$	2.390 (6)	2.375 (3)
Pb2—O1	2.410 (6)	2.384 (3)
Pb2—O2	2.746 (6)	2.753 (3)
$\text{Pb2—O5}^{\text{vi}}$	2.956 (7)	2.981 (4)
$\text{Pb2—O4}^{\text{vii}}$	3.128 (7)	3.029 (3)
$\text{Pb2—O6}^{\text{iii}}$	3.176 (7)	3.164 (3)
$\text{Pb2—O5}^{\text{vii}}$	3.225 (7)	3.200 (4)
$\text{Pb2—O4}^{\text{vi}}$	3.276 (7)	3.455 (3)
Te1—O2	1.891 (6)	1.890 (2)
Te1—O3	1.901 (6)	1.878 (2)
Te1—O1	1.902 (6)	1.895 (3)
Cr1—O7	1.634 (7)	1.462 (3)
Cr1—O5	1.640 (7)	1.476 (3)
Cr1—O4	1.653 (7)	1.488 (3)
Cr1—O6	1.667 (7)	1.484 (3)

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

consequences for those Pb—O bonds where the corresponding atoms O4–O7 are involved. These Pb—O bonds differ by up to 0.20 Å. A more quantitative comparison of the two isotypic structures was made with the program *COMP-*

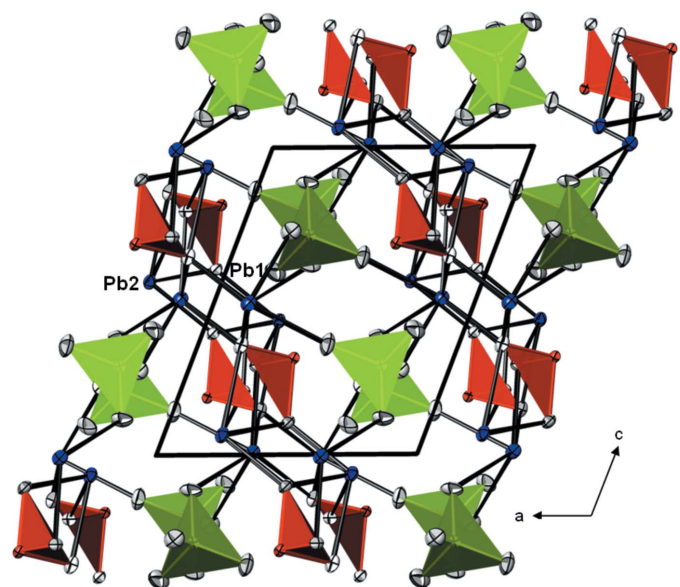


Figure 2
The crystal structure of $\text{Pb}_2(\text{CrO}_4)(\text{TeO}_3)$ in a projection along [010]. Te atoms and TeO_3^{2-} trigonal pyramids are given in red, CrO_4^{2-} tetrahedra in green, Pb^{2+} cations in blue, O atoms are colourless. For clarity, only Pb—O bonds < 2.8 Å are displayed. Displacement ellipsoids are given at the 50% probability level.

Table 2
Experimental details.

Crystal data	
Chemical formula	Pb ₂ (CrO ₄)(TeO ₃)
<i>M_r</i>	705.98
Crystal system, space group	Monoclinic, <i>P2₁/n</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.4736 (12), 10.8091 (16), 9.4065 (14)
β (°)	111.098 (12)
<i>V</i> (Å ³)	708.95 (19)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	52.91
Crystal size (mm)	0.09 × 0.06 × 0.01
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2015)
<i>T_{min}</i> , <i>T_{max}</i>	0.264, 0.494
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	23485, 2183, 1760
<i>R_{int}</i>	0.094
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.717
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.031, 0.070, 1.06
No. of reflections	2183
No. of parameters	100
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	2.47, -2.33

Computer programs: *APEX3* and *SAINT* (Bruker, 2015), *SHELXL2014* (Sheldrick, 2015), *ATOMS* (Dowty, 2006) and *publCIF* (Westrip, 2010).

STRU (de la Flor *et al.*, 2016). The degree of lattice distortion, *S*, is the spontaneous strain (sum of the squared eigenvalues of the strain tensor divided by 3) and amounts to 0.007. The maximum distance shows the maximal displacement between atomic positions of paired atoms and is 0.31 Å for atom pair O4. The next largest distances are 0.23 Å for pair O6, 0.17 Å for O5 and 0.13 Å for O7. The pairs of heavy atoms and the Cr/S pair show comparatively small distances of 0.095 Å (Pb1), 0.061 Å (Pb2), 0.087 Å (Te1) and 0.095 Å (Cr1/S1). The arithmetic mean of the distances is 0.12 Å. The measure of similarity (Δ) (Bergerhoff *et al.*, 1999) is 0.034, revealing a close relation between the two structures. Δ takes into consideration the differences in atomic positions and the ratios of the corresponding lattice parameters of the structures.

3. Synthesis and crystallization

Cr(NO₃)₃·9H₂O, PbF₂, PbO and TeO₂ were mixed thoroughly in a stoichiometric ratio of 1:1:2:1 and heated in an open alumina crucible to 1033 K within six h, held at this temperature for 30 h and cooled within eight h to room temperature. Most of the material had evaporated, and only a few orange plates of the title compound were left.

Alternatively, replacement of Cr(NO₃)₃·9H₂O with Cr₂O₃ under the same reaction conditions likewise led to the formation of Pb₂(CrO₄)(TeO₃).

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Starting coordinates were taken from isotypic Pb₂(SO₄)(TeO₃) (Weil & Shir Khanlou, 2017). The maximum and minimum electron densities are located 1.26 and 0.81 Å, respectively, from atom Pb2.

Acknowledgements

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Crystal structure of dilead(II) oxochromate(VI) oxotellurate(IV)

Matthias Weil

Computing details

Data collection: *APEX3* (Bruker, 2015); cell refinement: *SAINT* (Bruker, 2015); data reduction: *SAINT* (Bruker, 2015); program(s) used to solve structure: coordinates taken from an isotypic compound; program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ATOMS* (Dowty, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Dilead(II) oxochromate(VI) oxotellurate(IV)

Crystal data

$\text{Pb}_2(\text{CrO}_4)(\text{TeO}_3)$
 $M_r = 705.98$
 Monoclinic, $P2_1/n$
 $a = 7.4736$ (12) Å
 $b = 10.8091$ (16) Å
 $c = 9.4065$ (14) Å
 $\beta = 111.098$ (12)°
 $V = 708.95$ (19) Å³
 $Z = 4$

$F(000) = 1184$
 $D_x = 6.614$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 3031 reflections
 $\theta = 3.1\text{--}28.3^\circ$
 $\mu = 52.91$ mm⁻¹
 $T = 296$ K
 Plate, orange
 $0.09 \times 0.06 \times 0.01$ mm

Data collection

Bruker APEXII CCD
 diffractometer
 ω - and φ -scans
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2015)
 $T_{\min} = 0.264$, $T_{\max} = 0.494$
 23485 measured reflections

2183 independent reflections
 1760 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.094$
 $\theta_{\max} = 30.7^\circ$, $\theta_{\min} = 3.0^\circ$
 $h = -10 \rightarrow 10$
 $k = -15 \rightarrow 15$
 $l = -13 \rightarrow 13$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.070$
 $S = 1.06$
 2183 reflections
 100 parameters

0 restraints
 $w = 1/[\sigma^2(F_o^2) + (0.0264P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 2.47$ e Å⁻³
 $\Delta\rho_{\min} = -2.33$ e Å⁻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>	$U_{\text{iso}}^*/U_{\text{eq}}$
Pb1	0.86662 (5)	0.16252 (3)	0.49204 (4)	0.01746 (9)
Pb2	1.27667 (5)	0.45615 (3)	0.56450 (4)	0.01735 (9)
Te1	1.11378 (8)	0.63302 (5)	0.81301 (6)	0.01180 (12)
Cr1	1.2298 (2)	0.61161 (13)	1.21196 (16)	0.0152 (3)
O1	1.0417 (9)	0.5911 (6)	0.6035 (7)	0.0187 (13)
O2	1.3339 (8)	0.5323 (5)	0.8562 (7)	0.0159 (12)
O3	1.2413 (9)	0.7803 (5)	0.7920 (6)	0.0153 (12)
O4	1.3081 (10)	0.4675 (6)	1.2262 (8)	0.0295 (17)
O5	1.3146 (11)	0.6714 (6)	1.3836 (8)	0.0292 (16)
O6	1.3082 (11)	0.6927 (7)	1.0953 (8)	0.0331 (18)
O7	0.9957 (10)	0.6054 (7)	1.1419 (9)	0.0337 (18)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.01755 (19)	0.01525 (15)	0.01860 (18)	0.00102 (12)	0.00530 (14)	−0.00226 (12)
Pb2	0.01405 (18)	0.01770 (16)	0.01959 (18)	0.00177 (12)	0.00520 (14)	0.00440 (12)
Te1	0.0107 (3)	0.0117 (2)	0.0124 (3)	0.00001 (19)	0.0036 (2)	−0.00064 (19)
Cr1	0.0131 (7)	0.0191 (7)	0.0138 (7)	−0.0005 (5)	0.0053 (6)	−0.0002 (5)
O1	0.013 (3)	0.025 (3)	0.015 (3)	0.003 (3)	0.002 (3)	−0.004 (3)
O2	0.014 (3)	0.009 (3)	0.024 (3)	0.003 (2)	0.005 (3)	0.002 (2)
O3	0.018 (3)	0.013 (3)	0.014 (3)	−0.003 (2)	0.005 (3)	0.000 (2)
O4	0.032 (4)	0.024 (3)	0.031 (4)	0.003 (3)	0.010 (3)	−0.006 (3)
O5	0.041 (4)	0.028 (4)	0.018 (3)	0.007 (3)	0.010 (3)	−0.008 (3)
O6	0.040 (5)	0.036 (4)	0.029 (4)	−0.018 (3)	0.019 (4)	0.004 (3)
O7	0.017 (4)	0.039 (4)	0.043 (5)	0.005 (3)	0.010 (3)	0.015 (4)

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

Pb1—O2 ⁱ	2.429 (6)	Cr1—Te1 ^x	3.8465 (15)
Pb1—O3 ⁱⁱ	2.573 (6)	Cr1—Pb1 ^{xi}	3.9532 (15)
Pb1—O2 ⁱⁱⁱ	2.594 (6)	Cr1—Pb1 ^v	3.9593 (14)
Pb1—O7 ^{iv}	2.617 (7)	Cr1—Pb1 ^{xii}	4.1534 (15)
Pb1—O5 ^v	2.750 (7)	O1—Pb2 ⁱⁱ	2.390 (6)
Pb1—O4 ⁱ	2.777 (7)	O1—Pb1 ⁱⁱ	2.968 (6)
Pb1—O6 ⁱⁱⁱ	2.850 (7)	O1—Pb1 ^{xi}	4.515 (6)
Pb1—O1 ⁱⁱ	2.968 (6)	O2—Pb1 ^{xi}	2.429 (6)
Pb1—O3 ⁱⁱⁱ	3.170 (6)	O2—Pb1 ^{xii}	2.594 (6)
Pb1—Te1 ⁱⁱⁱ	3.6630 (9)	O2—Pb1 ⁱⁱ	4.508 (6)

Pb2—O3 ⁱⁱⁱ	2.363 (6)	O3—Pb2 ^{xii}	2.363 (6)
Pb2—O1 ⁱⁱ	2.390 (6)	O3—Pb1 ⁱⁱ	2.573 (6)
Pb2—O1	2.410 (6)	O3—Pb1 ^{xii}	3.170 (6)
Pb2—O2	2.746 (6)	O4—Pb1 ^{xi}	2.777 (7)
Pb2—O5 ^{vi}	2.956 (7)	O4—Pb2 ^{vii}	3.128 (7)
Pb2—O4 ^{vii}	3.128 (7)	O4—Te1 ^v	3.228 (7)
Pb2—O6 ⁱⁱⁱ	3.176 (7)	O4—Pb2 ^{ix}	3.276 (7)
Pb2—O5 ^{vii}	3.225 (7)	O4—Pb1 ^{xii}	4.262 (7)
Pb2—O4 ^{vi}	3.276 (7)	O5—Pb1 ^v	2.750 (7)
Pb2—Te1	3.5567 (7)	O5—Pb2 ^{ix}	2.956 (7)
Te1—O2	1.891 (6)	O5—Pb2 ^{vii}	3.225 (7)
Te1—O3	1.901 (6)	O5—Te1 ^x	3.314 (8)
Te1—O1	1.902 (6)	O6—Pb1 ^{xii}	2.850 (7)
Te1—O6	2.608 (7)	O6—Te1 ^x	3.097 (7)
Te1—O7 ^v	2.782 (7)	O6—Pb2 ^{xii}	3.176 (7)
Te1—O6 ^{viii}	3.097 (7)	O6—Pb2 ^{vii}	3.912 (8)
Cr1—O7	1.634 (7)	O6—Pb1 ^{xi}	4.023 (8)
Cr1—O5	1.640 (7)	O7—Pb1 ^{xiii}	2.617 (7)
Cr1—O4	1.653 (7)	O7—Te1 ^v	2.782 (7)
Cr1—O6	1.667 (7)	O7—Pb2 ^v	4.032 (8)
Cr1—Pb2 ^{vii}	3.6027 (16)	O7—Pb1 ^v	4.081 (8)
Cr1—Pb2 ^{ix}	3.6204 (15)	O7—Pb2 ^{ix}	4.099 (7)
Cr1—Te1 ^v	3.6339 (16)	O7—Pb1 ^{xi}	4.568 (8)
O2 ⁱ —Pb1—O3 ⁱⁱ	74.19 (19)	O7—Cr1—Pb1 ^{xi}	101.5 (3)
O2 ⁱ —Pb1—O2 ⁱⁱⁱ	73.9 (2)	O5—Cr1—Pb1 ^{xi}	136.8 (3)
O3 ⁱⁱ —Pb1—O2 ⁱⁱⁱ	126.0 (2)	O4—Cr1—Pb1 ^{xi}	35.4 (3)
O2 ⁱ —Pb1—O7 ^{iv}	69.6 (2)	O6—Cr1—Pb1 ^{xi}	80.3 (3)
O3 ⁱⁱ —Pb1—O7 ^{iv}	70.9 (2)	Te1—Cr1—Pb1 ^{xi}	60.35 (2)
O2 ⁱⁱⁱ —Pb1—O7 ^{iv}	132.5 (2)	Pb2 ^{vii} —Cr1—Pb1 ^{xi}	75.50 (3)
O2 ⁱ —Pb1—O5 ^v	144.9 (2)	Pb2 ^{ix} —Cr1—Pb1 ^{xi}	99.99 (3)
O3 ⁱⁱ —Pb1—O5 ^v	105.45 (19)	Te1 ^v —Cr1—Pb1 ^{xi}	74.38 (3)
O2 ⁱⁱⁱ —Pb1—O5 ^v	125.4 (2)	Te1 ^x —Cr1—Pb1 ^{xi}	110.89 (4)
O7 ^{iv} —Pb1—O5 ^v	77.1 (2)	O7—Cr1—Pb1 ^v	82.5 (3)
O2 ⁱ —Pb1—O4 ⁱ	87.9 (2)	O5—Cr1—Pb1 ^v	33.7 (3)
O3 ⁱⁱ —Pb1—O4 ⁱ	149.93 (19)	O4—Cr1—Pb1 ^v	132.3 (3)
O2 ⁱⁱⁱ —Pb1—O4 ⁱ	68.9 (2)	O6—Cr1—Pb1 ^v	109.6 (3)
O7 ^{iv} —Pb1—O4 ⁱ	80.3 (2)	Te1—Cr1—Pb1 ^v	131.89 (4)
O5 ^v —Pb1—O4 ⁱ	75.6 (2)	Pb2 ^{vii} —Cr1—Pb1 ^v	97.02 (3)
O2 ⁱ —Pb1—O6 ⁱⁱⁱ	83.2 (2)	Pb2 ^{ix} —Cr1—Pb1 ^v	67.93 (3)
O3 ⁱⁱ —Pb1—O6 ⁱⁱⁱ	69.8 (2)	Te1 ^v —Cr1—Pb1 ^v	101.01 (4)
O2 ⁱⁱⁱ —Pb1—O6 ⁱⁱⁱ	64.2 (2)	Te1 ^x —Cr1—Pb1 ^v	72.07 (3)
O7 ^{iv} —Pb1—O6 ⁱⁱⁱ	136.9 (2)	Pb1 ^{xi} —Cr1—Pb1 ^v	167.69 (4)
O5 ^v —Pb1—O6 ⁱⁱⁱ	130.5 (2)	O7—Cr1—Pb1 ^{xii}	132.0 (3)
O4 ⁱ —Pb1—O6 ⁱⁱⁱ	132.9 (2)	O5—Cr1—Pb1 ^{xii}	108.4 (3)
O2 ⁱ —Pb1—O1 ⁱⁱ	127.50 (19)	O4—Cr1—Pb1 ^{xii}	82.4 (3)
O3 ⁱⁱ —Pb1—O1 ⁱⁱ	59.35 (17)	O6—Cr1—Pb1 ^{xii}	30.7 (3)
O2 ⁱⁱⁱ —Pb1—O1 ⁱⁱ	113.96 (17)	Te1—Cr1—Pb1 ^{xii}	56.17 (2)

O7 ^{iv} —Pb1—O1 ⁱⁱ	112.2 (2)	Pb2 ^{vii} —Cr1—Pb1 ^{xii}	62.31 (3)
O5 ^v —Pb1—O1 ⁱⁱ	75.3 (2)	Pb2 ^{ix} —Cr1—Pb1 ^{xii}	129.63 (4)
O4 ⁱ —Pb1—O1 ⁱⁱ	144.43 (19)	Te1 ^v —Cr1—Pb1 ^{xii}	132.87 (4)
O6 ⁱⁱⁱ —Pb1—O1 ⁱⁱ	59.76 (19)	Te1 ^x —Cr1—Pb1 ^{xii}	54.39 (2)
O2 ⁱ —Pb1—O3 ⁱⁱⁱ	125.43 (18)	Pb1 ^{xi} —Cr1—Pb1 ^{xii}	59.33 (2)
O3 ⁱⁱ —Pb1—O3 ⁱⁱⁱ	116.15 (16)	Pb1 ^v —Cr1—Pb1 ^{xii}	126.12 (4)
O2 ⁱⁱⁱ —Pb1—O3 ⁱⁱⁱ	56.62 (16)	Te1—O1—Pb2 ⁱⁱ	125.4 (3)
O7 ^{iv} —Pb1—O3 ⁱⁱⁱ	164.00 (19)	Te1—O1—Pb2	110.6 (3)
O5 ^v —Pb1—O3 ⁱⁱⁱ	87.05 (19)	Pb2 ⁱⁱ —O1—Pb2	112.1 (2)
O4 ⁱ —Pb1—O3 ⁱⁱⁱ	93.90 (18)	Te1—O1—Pb1 ⁱⁱ	95.2 (2)
O6 ⁱⁱⁱ —Pb1—O3 ⁱⁱⁱ	56.72 (18)	Pb2 ⁱⁱ —O1—Pb1 ⁱⁱ	106.0 (2)
O1 ⁱⁱ —Pb1—O3 ⁱⁱⁱ	64.71 (16)	Pb2—O1—Pb1 ⁱⁱ	103.7 (2)
O2 ⁱ —Pb1—Te1 ⁱⁱⁱ	94.34 (14)	Te1—O1—Pb1 ^{xi}	55.69 (15)
O3 ⁱⁱ —Pb1—Te1 ⁱⁱⁱ	114.85 (13)	Pb2 ⁱⁱ —O1—Pb1 ^{xi}	121.5 (2)
O2 ⁱⁱⁱ —Pb1—Te1 ⁱⁱⁱ	29.32 (12)	Pb2—O1—Pb1 ^{xi}	63.04 (13)
O7 ^{iv} —Pb1—Te1 ⁱⁱⁱ	161.34 (16)	Pb1 ⁱⁱ —O1—Pb1 ^{xi}	132.40 (18)
O5 ^v —Pb1—Te1 ⁱⁱⁱ	116.07 (15)	Te1—O2—Pb1 ^{xi}	121.8 (3)
O4 ⁱ —Pb1—Te1 ⁱⁱⁱ	90.00 (15)	Te1—O2—Pb1 ^{xii}	108.5 (2)
O6 ⁱⁱⁱ —Pb1—Te1 ⁱⁱⁱ	45.10 (15)	Pb1 ^{xi} —O2—Pb1 ^{xii}	106.1 (2)
O1 ⁱⁱ —Pb1—Te1 ⁱⁱⁱ	84.89 (12)	Te1—O2—Pb2	98.5 (2)
O3 ⁱⁱⁱ —Pb1—Te1 ⁱⁱⁱ	31.26 (10)	Pb1 ^{xi} —O2—Pb2	102.47 (19)
O3 ⁱⁱⁱ —Pb2—O1 ⁱⁱ	87.6 (2)	Pb1 ^{xii} —O2—Pb2	120.4 (2)
O3 ⁱⁱⁱ —Pb2—O1	101.9 (2)	Te1—O2—Pb1 ⁱⁱ	52.16 (15)
O1 ⁱⁱ —Pb2—O1	67.9 (2)	Pb1 ^{xi} —O2—Pb1 ⁱⁱ	163.9 (2)
O3 ⁱⁱⁱ —Pb2—O2	72.00 (18)	Pb1 ^{xii} —O2—Pb1 ⁱⁱ	89.88 (14)
O1 ⁱⁱ —Pb2—O2	119.0 (2)	Pb2—O2—Pb1 ⁱⁱ	66.54 (12)
O1—Pb2—O2	61.76 (19)	Te1—O3—Pb2 ^{xii}	118.7 (3)
O3 ⁱⁱⁱ —Pb2—O5 ^{vi}	177.4 (2)	Te1—O3—Pb1 ⁱⁱ	109.1 (2)
O1 ⁱⁱ —Pb2—O5 ^{vi}	93.8 (2)	Pb2 ^{xii} —O3—Pb1 ⁱⁱ	109.8 (2)
O1—Pb2—O5 ^{vi}	80.6 (2)	Te1—O3—Pb1 ^{xii}	88.8 (2)
O2—Pb2—O5 ^{vi}	109.06 (17)	Pb2 ^{xii} —O3—Pb1 ^{xii}	100.75 (19)
O3 ⁱⁱⁱ —Pb2—O4 ^{vii}	95.8 (2)	Pb1 ⁱⁱ —O3—Pb1 ^{xii}	129.3 (2)
O1 ⁱⁱ —Pb2—O4 ^{vii}	176.63 (19)	Te1—O3—Pb2	58.39 (14)
O1—Pb2—O4 ^{vii}	110.89 (19)	Pb2 ^{xii} —O3—Pb2	176.2 (2)
O2—Pb2—O4 ^{vii}	61.95 (18)	Pb1 ⁱⁱ —O3—Pb2	73.89 (13)
O5 ^{vi} —Pb2—O4 ^{vii}	82.9 (2)	Pb1 ^{xii} —O3—Pb2	77.08 (11)
O3 ⁱⁱⁱ —Pb2—O6 ⁱⁱⁱ	60.41 (19)	Cr1—O4—Pb1 ^{xi}	124.4 (4)
O1 ⁱⁱ —Pb2—O6 ⁱⁱⁱ	60.90 (19)	Cr1—O4—Pb2 ^{vii}	92.6 (3)
O1—Pb2—O6 ⁱⁱⁱ	125.6 (2)	Pb1 ^{xi} —O4—Pb2 ^{vii}	103.2 (2)
O2—Pb2—O6 ⁱⁱⁱ	132.40 (18)	Cr1—O4—Te1 ^v	90.3 (3)
O5 ^{vi} —Pb2—O6 ⁱⁱⁱ	118.53 (18)	Pb1 ^{xi} —O4—Te1 ^v	99.5 (2)
O4 ^{vii} —Pb2—O6 ⁱⁱⁱ	121.22 (17)	Pb2 ^{vii} —O4—Te1 ^v	150.2 (3)
O3 ⁱⁱⁱ —Pb2—O5 ^{vii}	79.3 (2)	Cr1—O4—Pb2 ^{ix}	88.1 (3)
O1 ⁱⁱ —Pb2—O5 ^{vii}	132.23 (19)	Pb1 ^{xi} —O4—Pb2 ^{ix}	147.0 (2)
O1—Pb2—O5 ^{vii}	159.74 (19)	Pb2 ^{vii} —O4—Pb2 ^{ix}	78.49 (16)
O2—Pb2—O5 ^{vii}	100.28 (16)	Te1 ^v —O4—Pb2 ^{ix}	71.93 (15)
O5 ^{vi} —Pb2—O5 ^{vii}	98.15 (17)	Cr1—O4—Te1	60.7 (2)
O4 ^{vii} —Pb2—O5 ^{vii}	49.20 (17)	Pb1 ^{xi} —O4—Te1	64.28 (14)

O6 ⁱⁱⁱ —Pb2—O5 ^{vii}	72.86 (18)	Pb2 ^{vii} —O4—Te1	114.8 (2)
O3 ⁱⁱⁱ —Pb2—O4 ^{vi}	128.57 (18)	Te1 ^v —O4—Te1	92.34 (16)
O1 ⁱⁱ —Pb2—O4 ^{vi}	76.61 (19)	Pb2 ^{ix} —O4—Te1	145.4 (2)
O1—Pb2—O4 ^{vi}	115.84 (19)	Cr1—O4—Pb1 ^{xii}	75.0 (3)
O2—Pb2—O4 ^{vi}	156.81 (17)	Pb1 ^{xi} —O4—Pb1 ^{xii}	65.68 (15)
O5 ^{vi} —Pb2—O4 ^{vi}	49.92 (17)	Pb2 ^{vii} —O4—Pb1 ^{xii}	64.16 (13)
O4 ^{vii} —Pb2—O4 ^{vi}	101.51 (16)	Te1 ^v —O4—Pb1 ^{xii}	144.5 (2)
O6 ⁱⁱⁱ —Pb2—O4 ^{vi}	69.25 (17)	Pb2 ^{ix} —O4—Pb1 ^{xii}	137.7 (2)
O5 ^{vii} —Pb2—O4 ^{vi}	76.56 (18)	Te1—O4—Pb1 ^{xii}	52.26 (9)
O3 ⁱⁱⁱ —Pb2—Te1	87.36 (14)	Cr1—O5—Pb1 ^v	126.9 (4)
O1 ⁱⁱ —Pb2—Te1	93.13 (15)	Cr1—O5—Pb2 ^{ix}	100.0 (3)
O1—Pb2—Te1	30.03 (14)	Pb1 ^v —O5—Pb2 ^{ix}	96.0 (2)
O2—Pb2—Te1	31.73 (12)	Cr1—O5—Pb2 ^{vii}	89.4 (3)
O5 ^{vi} —Pb2—Te1	94.68 (13)	Pb1 ^v —O5—Pb2 ^{vii}	143.1 (2)
O4 ^{vii} —Pb2—Te1	86.63 (13)	Pb2 ^{ix} —O5—Pb2 ^{vii}	81.85 (17)
O6 ⁱⁱⁱ —Pb2—Te1	137.38 (13)	Cr1—O5—Te1 ^x	95.9 (3)
O5 ^{vii} —Pb2—Te1	131.31 (12)	Pb1 ^v —O5—Te1 ^x	98.0 (2)
O4 ^{vi} —Pb2—Te1	141.21 (12)	Pb2 ^{ix} —O5—Te1 ^x	146.0 (3)
O2—Te1—O3	94.3 (3)	Pb2 ^{vii} —O5—Te1 ^x	68.42 (15)
O2—Te1—O1	89.2 (3)	Cr1—O6—Te1	109.9 (3)
O3—Te1—O1	93.3 (3)	Cr1—O6—Pb1 ^{xii}	131.9 (4)
O2—Te1—O6	78.5 (3)	Te1—O6—Pb1 ^{xii}	84.2 (2)
O3—Te1—O6	77.4 (2)	Cr1—O6—Te1 ^x	103.6 (3)
O1—Te1—O6	163.8 (2)	Te1—O6—Te1 ^x	146.3 (3)
O2—Te1—O7 ^v	73.4 (2)	Pb1 ^{xii} —O6—Te1 ^x	75.99 (17)
O3—Te1—O7 ^v	167.7 (2)	Cr1—O6—Pb2 ^{xii}	136.5 (4)
O1—Te1—O7 ^v	87.0 (2)	Te1—O6—Pb2 ^{xii}	78.27 (18)
O6—Te1—O7 ^v	99.2 (2)	Pb1 ^{xii} —O6—Pb2 ^{xii}	90.68 (17)
O2—Te1—O6 ^{viii}	150.4 (2)	Te1 ^x —O6—Pb2 ^{xii}	75.03 (16)
O3—Te1—O6 ^{viii}	72.5 (2)	Cr1—O6—Pb2 ^{vii}	67.0 (2)
O1—Te1—O6 ^{viii}	66.0 (2)	Te1—O6—Pb2 ^{vii}	135.9 (3)
O6—Te1—O6 ^{viii}	122.06 (13)	Pb1 ^{xii} —O6—Pb2 ^{vii}	71.42 (16)
O7 ^v —Te1—O6 ^{viii}	118.5 (2)	Te1 ^x —O6—Pb2 ^{vii}	61.99 (13)
O7—Cr1—O5	113.0 (4)	Pb2 ^{xii} —O6—Pb2 ^{vii}	136.1 (2)
O7—Cr1—O4	106.9 (4)	Cr1—O6—Pb1 ^{xi}	75.6 (3)
O5—Cr1—O4	106.9 (3)	Te1—O6—Pb1 ^{xi}	65.61 (16)
O7—Cr1—O6	109.6 (4)	Pb1 ^{xii} —O6—Pb1 ^{xi}	69.10 (16)
O5—Cr1—O6	109.8 (4)	Te1 ^x —O6—Pb1 ^{xi}	128.5 (2)
O4—Cr1—O6	110.5 (4)	Pb2 ^{xii} —O6—Pb1 ^{xi}	139.7 (2)
O7—Cr1—Te1	76.0 (3)	Pb2 ^{vii} —O6—Pb1 ^{xi}	71.46 (13)
O5—Cr1—Te1	151.4 (3)	Cr1—O7—Pb1 ^{xiii}	163.1 (4)
O4—Cr1—Te1	95.3 (3)	Cr1—O7—Te1 ^v	107.9 (3)
O6—Cr1—Te1	43.8 (3)	Pb1 ^{xiii} —O7—Te1 ^v	89.0 (2)
O7—Cr1—Pb2 ^{vii}	161.7 (3)	Cr1—O7—Te1	77.3 (3)
O5—Cr1—Pb2 ^{vii}	63.5 (3)	Pb1 ^{xiii} —O7—Te1	95.7 (2)
O4—Cr1—Pb2 ^{vii}	60.2 (3)	Te1 ^v —O7—Te1	113.1 (2)
O6—Cr1—Pb2 ^{vii}	87.8 (3)	Cr1—O7—Pb2 ^v	117.5 (3)
Te1—Cr1—Pb2 ^{vii}	116.13 (4)	Pb1 ^{xiii} —O7—Pb2 ^v	71.26 (16)

O7—Cr1—Pb2 ^{ix}	95.0 (3)	Te1 ^v —O7—Pb2 ^v	59.62 (13)
O5—Cr1—Pb2 ^{ix}	53.5 (3)	Te1—O7—Pb2 ^v	164.5 (2)
O4—Cr1—Pb2 ^{ix}	64.8 (3)	Cr1—O7—Pb1 ^v	74.1 (3)
O6—Cr1—Pb2 ^{ix}	154.9 (3)	Pb1 ^{xiii} —O7—Pb1 ^v	99.4 (2)
Te1—Cr1—Pb2 ^{ix}	155.08 (4)	Te1 ^v —O7—Pb1 ^v	116.1 (2)
Pb2 ^{vii} —Cr1—Pb2 ^{ix}	68.28 (3)	Te1—O7—Pb1 ^v	128.5 (2)
O7—Cr1—Te1 ^v	46.7 (3)	Pb2 ^v —O7—Pb1 ^v	63.88 (12)
O5—Cr1—Te1 ^v	111.3 (3)	Cr1—O7—Pb2 ^{ix}	61.6 (2)
O4—Cr1—Te1 ^v	62.7 (3)	Pb1 ^{xiii} —O7—Pb2 ^{ix}	129.8 (2)
O6—Cr1—Te1 ^v	138.4 (3)	Te1 ^v —O7—Pb2 ^{ix}	64.15 (14)
Te1—Cr1—Te1 ^v	94.66 (4)	Te1—O7—Pb2 ^{ix}	133.03 (19)
Pb2 ^{vii} —Cr1—Te1 ^v	116.17 (4)	Pb2 ^v —O7—Pb2 ^{ix}	58.65 (10)
Pb2 ^{ix} —Cr1—Te1 ^v	63.55 (3)	Pb1 ^v —O7—Pb2 ^{ix}	62.50 (11)
O7—Cr1—Te1 ^x	136.4 (3)	Cr1—O7—Pb1 ^{xi}	58.0 (2)
O5—Cr1—Te1 ^x	59.0 (3)	Pb1 ^{xiii} —O7—Pb1 ^{xi}	129.7 (2)
O4—Cr1—Te1 ^x	116.4 (3)	Te1 ^v —O7—Pb1 ^{xi}	72.81 (16)
O6—Cr1—Te1 ^x	51.5 (3)	Te1—O7—Pb1 ^{xi}	53.91 (10)
Te1—Cr1—Te1 ^x	95.23 (3)	Pb2 ^v —O7—Pb1 ^{xi}	128.24 (17)
Pb2 ^{vii} —Cr1—Te1 ^x	59.04 (2)	Pb1 ^v —O7—Pb1 ^{xi}	130.79 (17)
Pb2 ^{ix} —Cr1—Te1 ^x	106.81 (4)	Pb2 ^{ix} —O7—Pb1 ^{xi}	83.91 (12)
Te1 ^v —Cr1—Te1 ^x	170.10 (4)		

Symmetry codes: (i) $x-1/2, -y+1/2, z-1/2$; (ii) $-x+2, -y+1, -z+1$; (iii) $-x+5/2, y-1/2, -z+3/2$; (iv) $-x+3/2, y-1/2, -z+3/2$; (v) $-x+2, -y+1, -z+2$; (vi) $x, y, z-1$; (vii) $-x+3, -y+1, -z+2$; (viii) $x-1/2, -y+3/2, z-1/2$; (ix) $x, y, z+1$; (x) $x+1/2, -y+3/2, z+1/2$; (xi) $x+1/2, -y+1/2, z+1/2$; (xii) $-x+5/2, y+1/2, -z+3/2$; (xiii) $-x+3/2, y+1/2, -z+3/2$.