A new oxyfluorotellurate(IV), InTe₂O₅F

Nefla Jennene Boukharrata, Jean-René Duclère, Jean-Paul Laval* and Philippe Thomas

Science des Procédés Céramiques et de Traitements de Surface, UMR-CNRS No. 7315, Université de Limoges, Centre Européen de la Céramique, 12 Rue Atlantis, 87068 Limoges Cedex, France

Correspondence e-mail: jean-paul.laval@unilim.fr

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A new oxyfluorotellurate(IV), indium fluoridopentaoxido-tellurate(IV), InTe₂O₅F, has been synthesized by solid-state reaction and structurally characterized. The crystal structure consists of a three-dimensional framework formed by InO₄F₂ octahedra and Te₂O₅ units. The InO₄F₂ octahedra are linked through the F atoms, which lie on twofold axes, giving rise to helical chains. These helical chains are connected *via* the Te₂O₅ units. The helical chains of indium octahedra surround cavities, into which the lone pairs of electrons of the Te atoms point.

Comment

Tellurates(IV) and selenates(IV) have attracted attention because of their ability to adopt a variety of structures in which the lone electron pair of the Te^{IV} and Se^{IV} cations may act as a structure-guiding agent (Berdonov *et al.*, 2009). Recently, the crystal structures of several oxyfluorotellurates(IV) showing a wide structural diversity [MTeO₃F (*M* = Fe^{III}, Ga^{III} and Cr^{III}; Laval *et al.*, 2008), ScTeO₃F and InTeO₃F (Jennene Boukharrata *et al.*, 2008), In₃TeO₃F₇ (Jennene Boukharrata *et al.*, 2011), and V₂Te₂O₇F₂ and TiTeO₃F₂ (Laval *et al.*, 2009)] have been described. The common characteristic of these structures is the presence of TeO₃*E* pyramids, where *E* represents a lone pair.

The present work is a continuation of our systematic investigation of tellurium(IV) fluorides and oxyfluorides. This work is directed to the synthesis of new phases of potential interest for their nonlinear optical properties and the characterization of new structure types, in order to determine the influence of the lone pair of electrons of the Te^{IV} cation on their structures. We are particularly interested in fluoride and oxyfluoride compounds, which are very sensitive to the stereochemical activity of this lone electron pair *E*. For oxyfluorides, the O/F anionic short- or long-range ordering has an important influence on the air stability of the compounds. In the In–Te–O–F system, two new structure types have been described previously, *viz.* InTeO₃F (Jennene Boukharrata *et*

al., 2008) and In₃TeO₃F₇ (Jennene Boukharrata *et al.*, 2011). In the present work, we report the synthesis and crystal structure determination of a new oxyfluorotellurate(IV) which is richer in tellurium, namely InTe₂O₅F.

The In atom of InTe₂O₅F occupies a slightly distorted octahedron. The equatorial apices of this octahedron are occupied by four O atoms (O1, O2ⁱ, O3ⁱⁱⁱ and O5) and the axial positions are occupied by the two F atoms (F1 and F2). Details of the In–O and In–F bond lengths are given in Table 1.

The Te atoms in the title structure occupy two different sites. Atom Te1 is strongly bonded to three O atoms (O3^{iv}, O4 and O5^{iv}; Table 1) and atom Te2 also has strong bonds to three O atoms (O1, O2 and O4; details in Table 1). The coordination polyhedra of the Te atoms are trigonal pyramids in both cases, with the stereochemically active electron lone pair *E* pointing in the direction of the fourth corner (Fig. 1).

When medium and long Te–O contacts are included in the coordination spheres, the descriptions of the environments of Te1 and Te2 change. One further Te–O bond can be added to the anionic environment of Te1 (Te1–O1ⁱⁱⁱ; Table 1), whereas three long Te–O bonds can be added to that of Te2 (Te2–O2^v, Te2–O3^{vi} and Te2–O4^{vi}; Table 1). Thus, the Te1O₄*E* polyhedron can be considered as a trigonal bipyramid, in which the third position in the equatorial plane is occupied by the lone pair *E*. This anionic environment can also be described as a disphenoid. The Te2O₆*E* polyhedron can be described as a distorted octahedron. The lone pair *E* points through the large triangular face of the octahedron (Fig. 1).

Atom O4 is shared by Te1 and Te2, forming a strong dinuclear [Te₂O₅]^{2–} unit (Fig. 1). However, considering the intermediate Te–O distances [for example, Te1–O1ⁱⁱⁱ = 2.369 (3) Å], the [Te₂O₅]^{2–} units are not isolated, but form part of [Te₂O₅]_∞ chains parallel to the (001) plane and oriented along the [110] and $\bar{1}10$ directions (Fig. 2). In these chains, the Te atoms have two different coordinations, *viz.* 3+1 for Te1 and 3 for Te2. This type of chain is also encountered in other compounds, such as CuTe₂O₅ (Hanke *et al.*, 1973) and Ga₂Te₄O₁₁ (Dutheil *et al.*, 2001).

Figure 1

The [Te₂O₅]^{2–} unit of the title compound. The arrows represent the lone electron pairs *E* of atoms Te1 and Te2. Short Te–O bonds are represented by continuous lines, and mid-range length and long Te–O bonds by dashed lines. [Symmetry codes: (iii) $x - \frac{1}{2}, y - \frac{1}{2}, z$; (iv) $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (v) $-x, y, -z + \frac{3}{2}$; (vi) $x, -y + 1, -z + 1$.]

Figure 2

The $[\text{Te}_2\text{O}_5]_\infty$ chains of the title compound. Dashed lines indicate mid-range Te—O bonds.

Bond-valence calculations (Brown, 1981) show that the O-atom valences range from 1.99 to 2.30 valence units (v.u.), and that the F-atom valences are 0.85 and 0.75 v.u. (Table 2). The calculated valences of the In, Te1 and Te2 atoms are very close to their theoretical values, which is consistent with full O/F ordering in the $\text{InTe}_2\text{O}_5\text{F}$ phase.

The $\text{InTe}_2\text{O}_5\text{F}$ octahedra share atoms F1 and F2, both of which lie on crystallographic twofold symmetry axes, to give $\text{In}_n\text{O}_{4n}\text{F}_n$ helical chains along the $[001]$ direction (Fig. 3). This kind of chain is found in other compounds containing indium, like $\text{NH}_4\text{In}(\text{OH})\text{PO}_4$ (Mao *et al.*, 2002) and $\text{KIn}(\text{OH})\text{PO}_4$ (Hriljac *et al.*, 1996), and also in $\gamma\text{-NaTiOPO}_4$ (Nagornyi *et al.*, 1989). Similar helical chains are also seen in $\text{BaMo}_2\text{Te}_2\text{O}_{11}(\text{H}_2\text{O})$ (Hou *et al.*, 2006), where the Mo atom is hexavalent (Mo^{6+}). Atoms Te1 and Te2 link the indium chains to give a three-dimensional framework. Indeed, in Fig. 3 it can be observed that the Te1 atoms share two O atoms (O5 and O3) with two In atoms belonging to two different helical chains. The third O atom (O4) is shared with atom Te2. The latter shares two O atoms (O1 and O2) with two In atoms belonging to the same helical chain. Therefore, each $[\text{Te}_2\text{O}_5]^{2-}$ unit links three different helical chains, two of which lie in the same (010) plane, while the third is shifted by $(x + \frac{1}{2}, y + \frac{1}{2})$.

A projection onto the (001) plane (Fig. 4) illustrates the cavities delimited by the helical shape of the indium chains and towards which the *E* lone pairs of the Te atoms point.

In this oxyfluorotellurate(IV), as in many Ga, Fe, Cr, V, Ti, In *etc.* oxyfluorotellurates already described, the bonding of the F atoms only to In ensures good thermal stability and nonhygroscopic character, due to the absence of unstable Te—F bonds.

The In—Te^{IV}—O—F system is the richest of the crystalline phases of the $M\text{—Te}^{\text{IV}}\text{—O—F}$ systems already studied. InTeO_3F (Jennene Boukharrata *et al.*, 2008), derived from the $\alpha\text{-PbO}_2$

Figure 3

Bridging of helical $\text{In}_n\text{O}_{4n}\text{F}_n$ chains by $[\text{Te}_2\text{O}_5]^{2-}$ units. Key: large dark balls (dark blue in the electronic version of the paper) are Te1 atoms and large light balls (light blue) are Te2 atoms. Atom labels are for general orientation purposes and do not include symmetry labels.

structure type, and $\text{In}_3\text{TeO}_3\text{F}_7$ (Jennene Boukharrata *et al.*, 2011) can be considered as intergrowths of $M\text{In}_3\text{F}_{10}$ and HTB (hexagonal tungsten bronze) types. $\text{InTe}_2\text{O}_5\text{F}$ is structurally

Figure 4

A projection of the $\text{InTe}_2\text{O}_5\text{F}$ structure onto the (001) plane, showing the cavities towards which the lone pairs *E* of the Te atoms point. Te1 atoms are shown as large dark balls (dark blue in the electronic version of the paper) and Te2 atoms are large light balls (light blue).

closer to classical tellurate(IV) structures but seems original due to the presence of helical chains of InO_4F_2 octahedra sharing F atoms connected through dinuclear $[\text{Te}_2\text{O}_5]^{2-}$ units, forming a three-dimensional framework. An investigation of the potential nonlinear optical properties of this noncentrosymmetric phase is planned.

Experimental

$\text{InTe}_2\text{O}_5\text{F}$ was prepared by solid-state reaction. InF_3 was obtained from Aldrich (99.9%) and TeO_2 was prepared by decomposition of commercial orthotelluric acid (H_6TeO_6 ; Aldrich, 99.9%). A mixture of InF_3 and TeO_2 (1:2.5 molar ratio) was ground in an agate mortar and quickly loaded into a platinum tube. The tube was sealed and heated as follows: the temperature was increased from 298 to 673 K (at a rate of 5 K min^{-1}), held there for 48 h and then decreased (at a rate of 0.1 K min^{-1}) to 573 K in intervals of 20 K. At the end of each interval the temperature was held fixed for 48 h. Colourless tablet-shaped single crystals of $\text{InTe}_2\text{O}_5\text{F}$, which were air-stable and suitable for study by X-ray diffraction, were obtained.

Crystal data

$\text{InTe}_2\text{O}_5\text{F}$	$V = 1029.9 (5) \text{ \AA}^3$
$M_r = 469.02$	$Z = 8$
Orthorhombic, $C222_1$	Mo $K\alpha$ radiation
$a = 6.964 (2) \text{ \AA}$	$\mu = 15.66 \text{ mm}^{-1}$
$b = 11.300 (3) \text{ \AA}$	$T = 293 \text{ K}$
$c = 13.088 (4) \text{ \AA}$	$0.02 \times 0.02 \times 0.01 \text{ mm}$

Data collection

Nonius KappaCCD area-detector diffractometer	15068 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2001)	1176 independent reflections
$T_{\min} = 0.754$, $T_{\max} = 0.829$	1113 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.044$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.015$	$\Delta\rho_{\text{max}} = 0.69 \text{ e \AA}^{-3}$
$wR(F^2) = 0.024$	$\Delta\rho_{\text{min}} = -0.72 \text{ e \AA}^{-3}$
$S = 1.13$	Absolute structure: Flack (1983),
1176 reflections	489 Friedel pairs
84 parameters	Flack parameter: $-0.01 (3)$

Data collection: *COLLECT* (Nonius, 2004); cell refinement: *DIRAX/LSQ* (Duisenberg *et al.*, 2003); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) and *WinGX* (Farrugia, 2012); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FN3131). Services for accessing these data are described at the back of the journal.

Table 1

Selected bond lengths ($\text{\AA}$).

In1—O1	2.133 (3)	Te1—O4	1.975 (3)
In1—O2 ⁱ	2.112 (3)	Te1—O5 ^{iv}	1.851 (3)
In1—O3 ⁱⁱ	2.140 (3)	Te2—O1	1.890 (3)
In1—O5	2.100 (3)	Te2—O2	1.854 (3)
In1—F1	2.1068 (17)	Te2—O2 ^v	2.710 (3)
In1—F2	2.1565 (16)	Te2—O3 ^{vi}	2.694 (3)
Te1—O1 ⁱⁱⁱ	2.369 (3)	Te2—O4	1.895 (3)
Te1—O3 ^{iv}	1.858 (3)	Te2—O4 ^{vi}	3.074 (3)

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

Table 2

Bond valences (v.u.) for $\text{InTe}_2\text{O}_5\text{F}$.

v_i denotes the bond-valence sum.

Atom	In1	Te1	Te2	v_i
O1	0.536	0.347	1.265	2.15
O2	0.567		1.394/0.138	2.10
O3	0.526	1.379	0.144	2.05
O4		1.005	1.248/0.052	2.30
O5	0.586	1.406		1.99
F1	0.427			0.85
F2	0.373			0.75
v_i	3.02	4.14	4.24	

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supplementary materials

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A new oxyfluorotellurate(IV), $\text{InTe}_2\text{O}_5\text{F}$

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Indium pentaoxidofluoridotellurate(IV)

Crystal data

$\text{InTe}_2\text{O}_5\text{F}$	$Z = 8$
$M_r = 469.02$	$F(000) = 1616$
Orthorhombic, $C222_1$	$D_x = 6.050 \text{ Mg m}^{-3}$
Hall symbol: C 2c 2	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 6.964 (2) \text{ \AA}$	$\mu = 15.66 \text{ mm}^{-1}$
$b = 11.300 (3) \text{ \AA}$	$T = 293 \text{ K}$
$c = 13.088 (4) \text{ \AA}$	Tablet, colourless
$V = 1029.9 (5) \text{ \AA}^3$	$0.02 \times 0.02 \times 0.01 \text{ mm}$

Data collection

Nonius KappaCCD raea-detector	$T_{\min} = 0.754, T_{\max} = 0.829$
diffractometer	15068 measured reflections
Radiation source: fine-focus sealed tube	1176 independent reflections
Horizontally mounted graphite crystal	1113 reflections with $I > 2\sigma(I)$
monochromator	$R_{\text{int}} = 0.044$
Detector resolution: 9 pixels mm^{-1}	$\theta_{\max} = 27.5^\circ, \theta_{\min} = 5.8^\circ$
CCD scans	$h = -8 \rightarrow 9$
Absorption correction: multi-scan	$k = -14 \rightarrow 14$
(<i>SADABS</i> ; Bruker, 2001)	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0082P)^2 + 1.3622P]$
Least-squares matrix: full	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.015$	$(\Delta/\sigma)_{\max} = 0.001$
$wR(F^2) = 0.024$	$\Delta\rho_{\max} = 0.69 \text{ e \AA}^{-3}$
$S = 1.13$	$\Delta\rho_{\min} = -0.72 \text{ e \AA}^{-3}$
1176 reflections	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $\text{Fc}^* = k\text{Fc}[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{-1/4}$
84 parameters	Extinction coefficient: 0.000384 (18)
0 restraints	Absolute structure: Flack (1983), 489 Friedel
Primary atom site location: structure-invariant	pairs
direct methods	Flack parameter: $-0.01 (3)$
Secondary atom site location: difference Fourier	
map	

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
In1	0.64821 (4)	0.40211 (3)	0.62646 (2)	0.00702 (8)
Te1	0.08894 (4)	0.23257 (3)	0.60885 (2)	0.00781 (7)
Te2	0.17699 (4)	0.55324 (3)	0.64544 (2)	0.00723 (8)
O1	0.4453 (4)	0.5435 (3)	0.6251 (2)	0.0106 (7)
O2	0.1843 (5)	0.5181 (3)	0.7838 (2)	0.0109 (7)
O3	0.3492 (4)	0.2343 (3)	0.3358 (2)	0.0102 (6)
O4	0.1389 (4)	0.4025 (3)	0.5854 (2)	0.0142 (7)
O5	0.5165 (4)	0.2813 (3)	0.5267 (2)	0.0109 (7)
F1	0.5000	0.3250 (3)	0.7500	0.0139 (9)
F2	0.7672 (6)	0.5000	0.5000	0.0182 (11)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
In1	0.00808 (15)	0.00621 (16)	0.00677 (15)	0.00056 (11)	−0.00022 (12)	−0.00067 (11)
Te1	0.00726 (13)	0.00863 (14)	0.00754 (14)	−0.00148 (12)	−0.00034 (12)	−0.00064 (12)
Te2	0.00774 (15)	0.00666 (16)	0.00730 (15)	0.00059 (11)	−0.00071 (12)	0.00030 (11)
O1	0.0071 (15)	0.0081 (16)	0.0165 (18)	−0.0002 (12)	0.0008 (14)	0.0003 (14)
O2	0.0115 (18)	0.0128 (18)	0.0085 (18)	0.0020 (15)	−0.0025 (14)	0.0040 (13)
O3	0.0086 (14)	0.0101 (16)	0.0120 (16)	−0.0022 (13)	−0.0024 (12)	−0.0006 (13)
O4	0.0185 (18)	0.0058 (17)	0.0184 (17)	−0.0059 (13)	0.0009 (14)	−0.0037 (14)
O5	0.0154 (17)	0.0104 (18)	0.0068 (16)	−0.0008 (15)	−0.0008 (13)	−0.0028 (15)
F1	0.012 (2)	0.012 (2)	0.018 (2)	0.000	0.0060 (16)	0.000
F2	0.010 (2)	0.031 (3)	0.013 (2)	0.000	0.000	0.0054 (18)

Geometric parameters ($\text{\AA}$, $^\circ$)

In1—O1	2.133 (3)	O2—O2 ^v	2.715 (7)
In1—O2 ⁱ	2.112 (3)	O2—O4	2.924 (5)
In1—O3 ⁱⁱ	2.140 (3)	O2—O3 ^{viii}	2.943 (5)
In1—O5	2.100 (3)	O2—O4 ^v	3.115 (4)
In1—F1	2.1068 (17)	O2—Te1 ^{ix}	3.215 (3)
In1—F2	2.1565 (16)	O3—Te1 ⁱⁱ	1.858 (3)
Te1—O1 ⁱⁱⁱ	2.369 (3)	O3—In1 ^{iv}	2.140 (3)
Te1—O3 ^{iv}	1.858 (3)	O3—Te2 ^{vi}	2.694 (3)
Te1—O4	1.975 (3)	O3—O4 ⁱⁱ	2.743 (4)
Te1—O5 ^{iv}	1.851 (3)	O3—O2 ^x	2.943 (5)
Te2—O1	1.890 (3)	O3—Te1 ^x	3.025 (3)
Te2—O2	1.854 (3)	O3—O3 ^{xi}	3.076 (6)
Te2—O2 ^v	2.710 (3)	O4—O3 ^{iv}	2.743 (4)
Te2—O3 ^{vi}	2.694 (3)	O4—Te2 ^{vi}	3.074 (3)
Te2—O4	1.895 (3)	O4—O2 ^v	3.115 (4)

Te2—O4 ^{vi}	3.074 (3)	O4—O4 ^{vi}	3.140 (6)
O1—Te1 ^{vii}	2.369 (3)	O5—Te1 ⁱⁱ	1.851 (3)
O2—In1 ⁱ	2.112 (3)	F1—In1 ⁱ	2.1068 (17)
O2—Te2 ^v	2.710 (3)	F2—In1 ^{vi}	2.1565 (16)
O5—In1—F1	89.68 (11)	In1 ⁱ —O2—O3 ^{viii}	46.60 (8)
O5—In1—O2 ⁱ	172.20 (12)	Te2 ^v —O2—O3 ^{viii}	89.38 (10)
F1—In1—O2 ⁱ	95.77 (11)	O2 ^v —O2—O3 ^{viii}	90.03 (9)
O5—In1—O1	101.10 (12)	O4—O2—O3 ^{viii}	76.31 (11)
F1—In1—O1	89.50 (12)	Te2—O2—O4 ^v	127.33 (16)
O2 ⁱ —In1—O1	84.57 (12)	In1 ⁱ —O2—O4 ^v	80.38 (11)
O5—In1—O3 ⁱⁱ	87.74 (12)	O2 ^v —O2—O4 ^v	59.72 (12)
F1—In1—O3 ⁱⁱ	81.10 (11)	O4—O2—O4 ^v	102.83 (14)
O2 ⁱ —In1—O3 ⁱⁱ	87.59 (12)	O3 ^{viii} —O2—O4 ^v	53.76 (9)
O1—In1—O3 ⁱⁱ	167.11 (11)	Te2—O2—Te1 ^{ix}	106.20 (12)
O5—In1—F2	91.38 (10)	In1 ⁱ —O2—Te1 ^{ix}	87.34 (11)
F1—In1—F2	171.69 (11)	Te2 ^v —O2—Te1 ^{ix}	101.32 (10)
O2 ⁱ —In1—F2	84.04 (11)	O2 ^v —O2—Te1 ^{ix}	127.35 (8)
O1—In1—F2	82.20 (11)	O4—O2—Te1 ^{ix}	141.08 (13)
O3 ⁱⁱ —In1—F2	107.17 (12)	O3 ^{viii} —O2—Te1 ^{ix}	131.95 (12)
O5 ^{iv} —Te1—O3 ^{iv}	98.37 (13)	O4 ^v —O2—Te1 ^{ix}	115.53 (11)
O5 ^{iv} —Te1—O4	88.94 (14)	Te1 ⁱⁱ —O3—In1 ^{iv}	130.00 (16)
O3 ^{iv} —Te1—O4	91.33 (14)	Te1 ⁱⁱ —O3—Te2 ^{vi}	100.67 (13)
O5 ^{iv} —Te1—O1 ⁱⁱⁱ	83.97 (13)	In1 ^{iv} —O3—Te2 ^{vi}	109.26 (11)
O3 ^{iv} —Te1—O1 ⁱⁱⁱ	76.52 (12)	Te1 ⁱⁱ —O3—O4 ⁱⁱ	46.04 (10)
O4—Te1—O1 ⁱⁱⁱ	164.83 (12)	In1 ^{iv} —O3—O4 ⁱⁱ	89.33 (12)
O5 ^{iv} —Te1—O3 ^{viii}	172.10 (11)	Te2 ^{vi} —O3—O4 ⁱⁱ	142.68 (13)
O3 ^{iv} —Te1—O3 ^{viii}	73.76 (12)	Te1 ⁱⁱ —O3—O2 ^x	110.88 (15)
O4—Te1—O3 ^{viii}	90.40 (11)	In1 ^{iv} —O3—O2 ^x	45.81 (9)
O1 ⁱⁱⁱ —Te1—O3 ^{viii}	94.78 (10)	Te2 ^{vi} —O3—O2 ^x	148.17 (13)
O5 ^{iv} —Te1—O2 ^{xii}	119.27 (12)	O4 ⁱⁱ —O3—O2 ^x	66.34 (11)
O3 ^{iv} —Te1—O2 ^{xii}	115.00 (11)	Te1 ⁱⁱ —O3—Te1 ^x	103.29 (11)
O4—Te1—O2 ^{xii}	135.54 (11)	In1 ^{iv} —O3—Te1 ^x	114.13 (11)
O1 ⁱⁱⁱ —Te1—O2 ^{xii}	59.23 (9)	Te2 ^{vi} —O3—Te1 ^x	92.45 (9)
O3 ^{viii} —Te1—O2 ^{xii}	66.05 (8)	O4 ⁱⁱ —O3—Te1 ^x	109.50 (11)
O2—Te2—O1	95.60 (15)	O2 ^x —O3—Te1 ^x	84.48 (10)
O2—Te2—O4	102.49 (14)	Te1 ⁱⁱ —O3—O3 ^{xi}	70.78 (11)
O1—Te2—O4	91.57 (14)	In1 ^{iv} —O3—O3 ^{xi}	127.96 (10)
O2—Te2—O3 ^{vi}	95.13 (12)	Te2 ^{vi} —O3—O3 ^{xi}	111.74 (7)
O1—Te2—O3 ^{vi}	67.98 (11)	O4 ⁱⁱ —O3—O3 ^{xi}	76.81 (12)
O4—Te2—O3 ^{vi}	154.30 (11)	O2 ^x —O3—O3 ^{xi}	83.40 (9)
O2—Te2—O2 ^v	70.15 (15)	Te2—O4—Te1	146.56 (18)
O1—Te2—O2 ^v	163.14 (12)	Te2—O4—O3 ^{iv}	117.00 (15)
O4—Te2—O2 ^v	83.12 (11)	Te1—O4—O2	108.42 (14)
O3 ^{vi} —Te2—O2 ^v	120.82 (9)	O3 ^{iv} —O4—O2	89.88 (12)
O2—Te2—O4 ^{vi}	175.52 (12)	Te2—O4—Te2 ^{vi}	104.42 (12)
O1—Te2—O4 ^{vi}	87.51 (11)	Te1—O4—Te2 ^{vi}	109.02 (12)
O4—Te2—O4 ^{vi}	74.15 (12)	O3 ^{iv} —O4—Te2 ^{vi}	121.63 (12)
O3 ^{vi} —Te2—O4 ^{vi}	89.02 (8)	O2—O4—Te2 ^{vi}	142.25 (12)

O2 ^v —Te2—O4 ^{vi}	106.24 (9)	Te2—O4—O2 ^v	59.74 (10)
Te2—O1—In1	134.23 (15)	Te1—O4—O2 ^v	101.26 (12)
Te2—O1—Te1 ^{vii}	112.17 (13)	O3 ^{iv} —O4—O2 ^v	59.90 (11)
In1—O1—Te1 ^{vii}	113.35 (12)	O2—O4—O2 ^v	53.32 (13)
Te2—O2—In1 ⁱ	133.72 (18)	Te2 ^{vi} —O4—O2 ^v	122.28 (12)
Te2—O2—Te2 ^v	106.08 (14)	Te2—O4—O4 ^{vi}	70.37 (12)
In1 ⁱ —O2—Te2 ^v	114.42 (12)	Te1—O4—O4 ^{vi}	142.44 (19)
Te2—O2—O2 ^v	69.88 (13)	O3 ^{iv} —O4—O4 ^{vi}	131.54 (9)
In1 ⁱ —O2—O2 ^v	134.70 (13)	O2—O4—O4 ^{vi}	108.58 (15)
In1 ⁱ —O2—O4	106.02 (13)	O2 ^v —O4—O4 ^{vi}	95.56 (11)
Te2 ^v —O2—O4	105.58 (13)	Te1 ⁱⁱ —O5—In1	122.13 (16)
O2 ^v —O2—O4	66.96 (12)	In1—F1—In1 ⁱ	131.1 (2)
Te2—O2—O3 ^{viii}	115.54 (15)	In1 ^{vi} —F2—In1	134.8 (2)

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

Bond valences (v.u.) for InTe₂O₅F [Define v_i?]

Atom	In1	Te1	Te2	v _i
O1	0.536	0.347	1.265	2.15
O2	0.567		1.394/0.138	2.10
O3	0.526	1.379	0.144	2.05
O4		1.005	1.248/0.052	2.30
O5	0.586	1.406		1.99
F1	0.427			0.85
F2	0.373			0.75
v _i	3.02	4.14	4.24	