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Tris[triphenylantimony(V)]hexa(μ -oxido)-tellurium(VI): a molecular complex with six Te—O—Sb bridges

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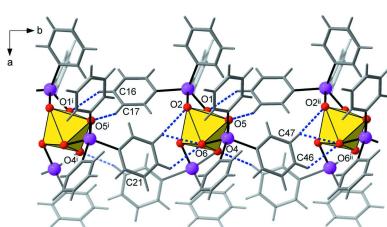
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In the structure of the title compound [systematic name hexa- μ -oxido- $1:2\kappa^4O:O:1:3\kappa^4O:O:1:4\kappa^4O:O$ -nonaphenyl- $2\kappa^3C,3\kappa^3C,4\kappa^3C$ -triantimony(V)tellurium(VI)], $[Sb_3Te(C_6H_5)_9O_6]$, the hexaoxidotellurate(VI) ion is coordinated to three Sb^V ions via pairs of *cis*-positioned O atoms to form a discrete molecular unit. The Te^{VI} and Sb^V central ions exhibit distorted octahedral $[TeO_6]$ and distorted trigonal-bipyramidal $[SbC_3O_2]$ coordination geometries, respectively. The linking of these polyhedra, by sharing the dioxide edges, results in the Te-based octahedron having a *mer*-configuration. The packing of the molecules is dominated by C—H···O hydrogen bonding and weak dispersion forces, with a minor contribution from C—H··· π bonds and π — π stacking interactions. According to the Hirshfeld surface analysis, the contributions of the H···H, H···C/C···H and H···O/O···H contacts are 58.0, 32.6 and 7.8%, respectively. The title structure provides a model for the bonding of triorganoantimony dication to octahedral oxoanions, and the observed doubly bridged motifs, Te(μ -O)₂Sb, may find application in the functionalization of polyoxometalate species.

1. Chemical context

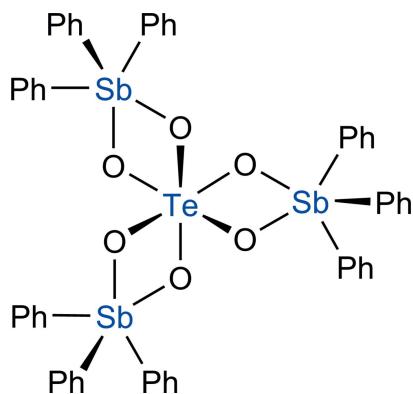
Organointimony(V) species readily form covalent derivatives with a range of organic and inorganic oxo-ions and these can be used in the construction of metal–oxide clusters (Nicholson *et al.*, 2011). Unlike the series of molecular fivefold-coordinated tetraphenylantimony(V) compounds, which easily dissociate in solution to yield tetraphenylstibonium cations, $[Ph_4Sb]^+$ (Domasevitch *et al.*, 2000), the derivatives of triphenylantimony(V) are much more chemically robust and they are well suited for the preparation of covalent oxide materials. The interactions between the Ph₃Sb²⁺ cations and oxoanions are particularly important as they potentially control the assembly of these units into either discrete oxo-clusters or polymers. For example, one-dimensional covalent chains of oxo-bridged Ph₃Sb²⁺ moieties were identified as a possible motif for amorphous $[Ph_3SbO]_n$ formation (Carmalt *et al.*, 1996). In addition, there are a few complexes known in which singly charged oxoanions form molecular five-coordinate structures with terminal $[ReO_4]^-$ (Wirringa *et al.*, 1992) or $[PhSO_3]^-$ (Rüther *et al.*, 1986) groups or bridging $[Ph_2PO_2]^-$ groups (Srungavruksham & Baskar, 2013), while insoluble derivatives with tetrahedral dianions, such as SO₄²⁻, SeO₄²⁻ and CrO₄²⁻, are likely to be polymeric (Goel *et al.*, 1969).

At the same time, Ph₃Sb²⁺ units may coordinate to the O atoms of octahedral oxoanion species to form discrete mol-



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ecules: one can anticipate using $\text{Ph}_3\text{Sb}^{2+}$ for the functionalization of inorganic metal–oxide octahedra with the generation of doubly bridged $M(\mu\text{-O})_2\text{Sb}$ motifs. The latter are formally similar to 1,2-benzenediolate chelates, which have been observed in molecular organoantimony compounds (Hall & Sowerby, 1980). Such double bridges are well suited for covalent immobilization of triorganoantimony moieties at the developed metal–oxide surfaces of polyoxometalates. The coordination behaviour of such systems, however, does not appear to have been considered so far. In this context, we have examined a structurally simple and attractive inorganic oxoanion, namely octahedral hexaoxidotellurate(VI). In the present contribution, we crystallize this unit with $\text{Ph}_3\text{Sb}^{2+}$ units and report the crystal structure of the title compound, $(\text{C}_{18}\text{H}_{15}\text{Sb})_3\text{TeO}_6$, which features the formation of discrete clusters, $[\text{Te}[(\mu\text{-O})_2\text{SbPh}_3]_3]$.



2. Structural commentary

The title compound crystallizes in the monoclinic space group $C2/c$, and contains the discrete molecular unit shown in Fig. 1.

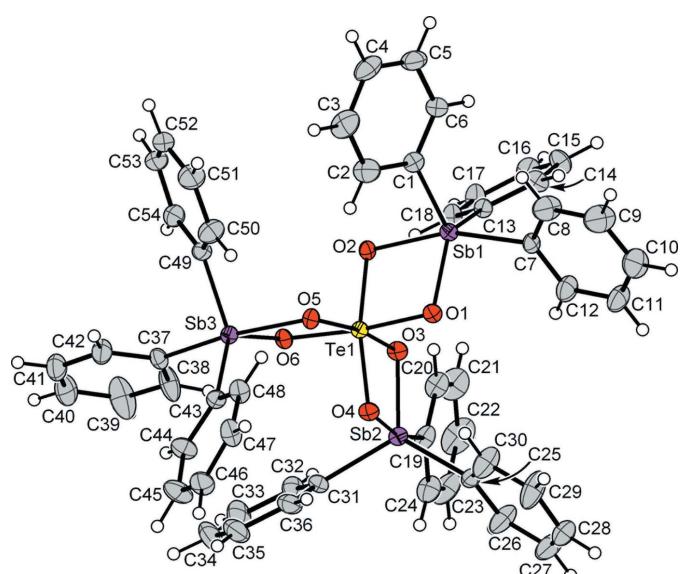


Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 40% probability level. Hydrogen atoms are represented by small circles of arbitrary radius.

Table 1
Selected geometric parameters (\AA , $^\circ$).

Te1—O2	1.904 (3)	Sb2—O3	1.966 (3)
Te1—O5	1.904 (3)	Sb2—O4	2.087 (3)
Te1—O4	1.918 (3)	Sb2—C25	2.136 (5)
Te1—O1	1.949 (3)	Sb2—C31	2.147 (5)
Te1—O6	1.964 (3)	Sb2—C19	2.170 (4)
Te1—O3	1.968 (3)	Sb3—O6	1.967 (3)
Sb1—O1	1.992 (3)	Sb3—O5	2.110 (3)
Sb1—O2	2.091 (3)	Sb3—C49	2.112 (5)
Sb1—C1	2.110 (5)	Sb3—C43	2.122 (4)
Sb1—C13	2.128 (4)	Sb3—C37	2.165 (4)
Sb1—C7	2.175 (4)		
O2—Te1—O5	97.67 (13)	O3—Sb2—C25	118.46 (16)
O2—Te1—O4	166.37 (13)	O4—Sb2—C25	88.80 (15)
O5—Te1—O4	94.67 (13)	O3—Sb2—C31	119.67 (17)
O2—Te1—O1	81.53 (12)	O4—Sb2—C31	87.58 (16)
O5—Te1—O1	95.83 (13)	C25—Sb2—C31	118.87 (19)
O4—Te1—O1	91.49 (13)	O3—Sb2—C19	88.62 (17)
O2—Te1—O6	94.01 (13)	O4—Sb2—C19	164.73 (16)
O5—Te1—O6	81.51 (12)	C25—Sb2—C19	101.04 (18)
O4—Te1—O6	93.53 (13)	C31—Sb2—C19	97.6 (2)
O1—Te1—O6	174.49 (13)	O6—Sb3—O5	76.45 (12)
O2—Te1—O3	88.47 (13)	O6—Sb3—C49	116.47 (16)
O5—Te1—O3	168.81 (13)	O5—Sb3—C49	89.13 (16)
O4—Te1—O3	80.35 (12)	O6—Sb3—C43	126.74 (16)
O1—Te1—O3	94.32 (13)	O5—Sb3—C43	87.41 (15)
O6—Te1—O3	88.77 (13)	C49—Sb3—C43	113.58 (18)
O1—Sb1—O2	76.01 (12)	O6—Sb3—C37	89.39 (16)
O1—Sb1—C1	119.50 (15)	O5—Sb3—C37	165.43 (16)
O2—Sb1—C1	91.35 (15)	C49—Sb3—C37	100.46 (19)
O1—Sb1—C13	124.71 (15)	C43—Sb3—C37	98.58 (17)
O2—Sb1—C13	91.45 (14)	Te1—O1—Sb1	102.08 (13)
C1—Sb1—C13	114.34 (17)	Te1—O2—Sb1	100.07 (13)
O1—Sb1—C7	85.22 (15)	Sb2—O3—Te1	102.41 (13)
O2—Sb1—C7	161.09 (15)	Te1—O4—Sb2	99.85 (12)
C1—Sb1—C7	99.99 (18)	Te1—O5—Sb3	99.33 (13)
C13—Sb1—C7	97.49 (17)	Te1—O6—Sb3	102.36 (14)
O3—Sb2—O4	76.38 (12)		

The asymmetric tetranuclear molecule comprises a $[\text{TeO}_6]$ octahedron and three $[\text{Ph}_3\text{SbO}_2]$ polyhedra sharing oxide edges. Thus two oxide bridges are formed from Te^{VI} to each of the three Sb^{V} ions with $\text{Te}—\text{O}—\text{Sb}$ angles in the range $99.33 (13)$ – $102.41 (13)^\circ$ (Table 1). The three $\text{Te}(\mu\text{-O})_2\text{Sb}$ rhombuses are nearly planar, with the maximum deviation of the Te atom from the corresponding mean plane being $0.0676 (12)$ \AA , which occurs in the $\text{Te}1(\mu\text{-O})_2\text{Sb}2$ unit. Such fully substituted organometallic hexaoxotellurate(VI) units are exceedingly rare, with the only known example being an aliphatic Sn^{IV} derivative (Beckmann *et al.*, 2002). In addition, only two triphenyltin(IV) analogues of the title compound are known, namely $[(\text{Ph}_3\text{SnO})_4\text{Te}(\text{OH})_2]$ and $[(\text{Ph}_3\text{SnO})_2\text{Te}(\text{OMe})_4]$ (Herntrich & Merzweiler, 2010).

The $\text{Te}1$ atom adopts a slightly distorted octahedral coordination, with the three *trans* $\text{O}—\text{Te}—\text{O}$ bond angles lying within the range $166.37 (13)$ – $174.49 (13)^\circ$. The fivefold coordination around each of three Sb-atoms can best be described as distorted trigonal bipyramidal, with the $\text{O}2—\text{Sb}1—\text{C}7 = 161.09 (15)^\circ$, $\text{O}4—\text{Sb}2—\text{C}19 = 164.73 (16)^\circ$ and $\text{O}5—\text{Sb}3—\text{C}37 = 165.43 (16)^\circ$ bond angles defining the principal axes of the trigonal bipyramids. This assignment is supported by the calculated five-coordinate τ -indices, which are 0.69, 0.75 and 0.65 for $\text{Sb}1$, $\text{Sb}2$ and $\text{Sb}3$, respectively

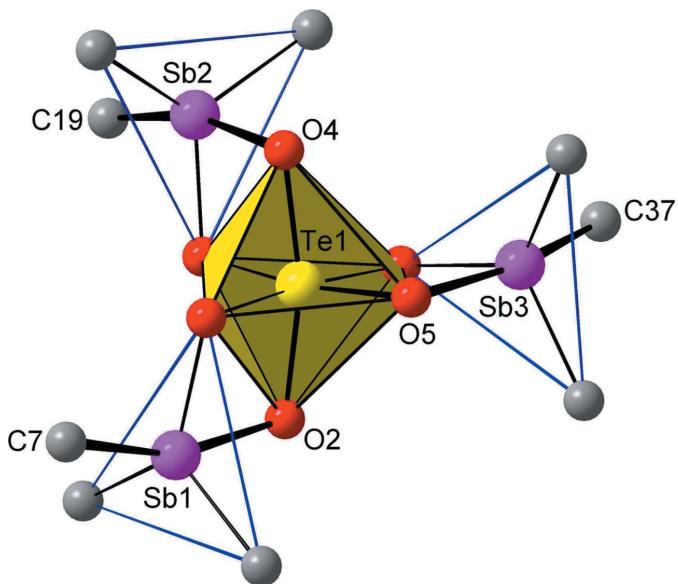


Figure 2

The connection of the Te- and Sb-coordination polyhedra, showing the *mer*-configuration of the $[TeO_6]$ octahedron in the environment of three $[Sb_3O_2]$ trigonal bipyramids. The principal axes of the trigonal bipyramids are marked with thick black bonds and their equatorial planes are indicated by blue lines.

(Addison *et al.*, 1984). These values are closer to unity, the value expected for a perfect trigonal-bipyramidal geometry, than to zero, which is expected for a square-based pyramidal geometry.

In each of the three Sb-based trigonal bipyramids, the axial Sb—O_{ax} bonds, Sb1—O2, Sb2—O4 and Sb3—O5, are slightly longer [in the range 2.087 (3)–2.110 (3) Å] than the equatorial Sb—O_{eq} bonds, Sb1—O1, Sb2—O3 and Sb3—O6 [in the range 1.966 (3)–1.992 (3) Å]. This observation coincides with the differentiation of the Te—O bond lengths; three of which, Te1—O2, Te1—O4 and Te1—O5, lie in the range 1.904 (3)–1.918 (3) Å and three, Te1—O1, Te1—O3 and Te1—O6, lie in the range 1.949 (3)–1.968 (3) Å. Thus when considering the six Te—O—Sb bridges, the shorter Sb—O bonds are accompanied by the longer Te—O bonds and *vice versa*. The distribution of the Te—O_{ax}Sb and Te—O_{eq}Sb bonds indicates that the coordination octahedron around the Te atom has the *mer*-configuration (Fig. 2). This is consistent with the *mer*-octahedral geometry adopted in the previously examined trisubstituted tellurates, *e.g.* *mer*-[(Bu₃SnO)₃Te(OH)₃] (Beckmann *et al.*, 2002).

3. Supramolecular features

The relatively loose packing of the title compound is dominated by weak dispersion forces, with the calculated packing index of 67.5 approaching the lower limit of the 65–75% range expected for organic solids (Dunitz, 1995). For comparison, the perceptibly denser packing of more symmetrical polyphenyl substituted species, *e.g.* 1,3,5,7-tetraphenyladamantane, supporting a complex framework of aromatic

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O1 ⁱ	0.95	2.58	3.342 (6)	137
C17—H17···O5 ⁱ	0.95	2.58	3.437 (6)	150
C21—H21···O4 ⁱ	0.95	2.75	3.651 (8)	158
C46—H46···O6 ⁱⁱ	0.95	2.67	3.276 (6)	122
C47—H47···O6 ⁱⁱ	0.95	2.73	3.307 (6)	120
C47—H47···O2 ⁱⁱ	0.95	2.70	3.645 (6)	177

Symmetry codes: (i) $x, y - 1, z$; (ii) $x, y + 1, z$.

interactions, has a packing index of 70.4 (Boldog *et al.*, 2009). In the absence of stronger bonding, the present supramolecular array is mediated by a series of C—H···O and C—H···π hydrogen bonds with a minor contribution from π/π stacking interactions.

Very weak mutual C—H···O bonding [with the shortest separation C46···O6ⁱⁱ = 3.276 (6) Å; symmetry code (ii) $x, y + 1, z$; Table 2] arranges the molecules into chains running parallel to the *b* direction (Fig. 3). Three out of the six above-mentioned interactions present are relatively directional, with the angles at the H atoms lying in the range 150–177°. Even weaker C—H···π interactions are observed between adjacent chains (Fig. 4). The two shortest of these are C11—H11···Cg(C43—C48)ⁱⁱⁱ and C41—H41···Cg(C13—C18)^{iv} (where Cg is a ring centroid; symmetry codes: (iii) $x, -y + 2, x - \frac{1}{2}$; (iv) $x, -y + 1, z + \frac{1}{2}$, with C···π separations of 3.775 (6) and 3.505 (6) Å and C—H···π angles of 137 and 124°, respectively. This bonding connects the chains into bilayers, which lie parallel to the *bc* plane. In addition, to further consolidate the bilayers, there are weak slipped π—π stacking interactions between pairs of inversion-related phenyl rings, with a centroid-to-centroid distance, Cg(C1—C6)···Cg(C1—C6)^v = 3.807 (6) Å, an interplanar distance of 3.603 (5) Å and a slippage angle of 18.8 (5)° [symmetry code: (v) $-x, -y + 1, -z$]. There are no specific interactions between the bilayers, and the shortest of their C···C contacts [3.404 (6) Å] is not accompanied by any π—π overlap.

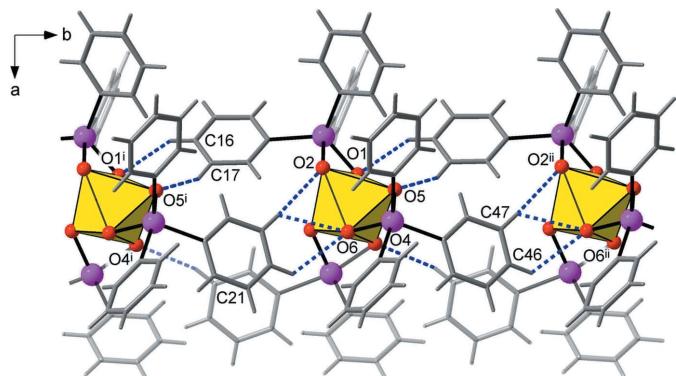
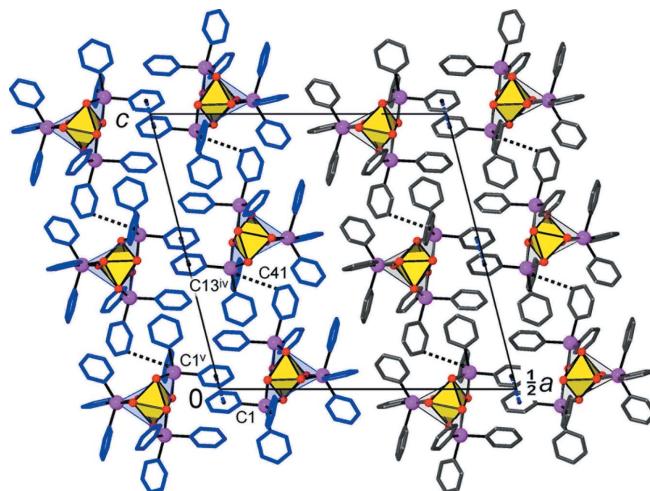


Figure 3

One-dimensional chains running along the *b*-axis direction, in which translation-related molecules of the title compound are linked by a series of weak C—H···O hydrogen bonds (shown as dashed blue lines). [Symmetry codes: (i) $x, y - 1, z$; (ii) $x, y + 1, z$.]

**Figure 4**

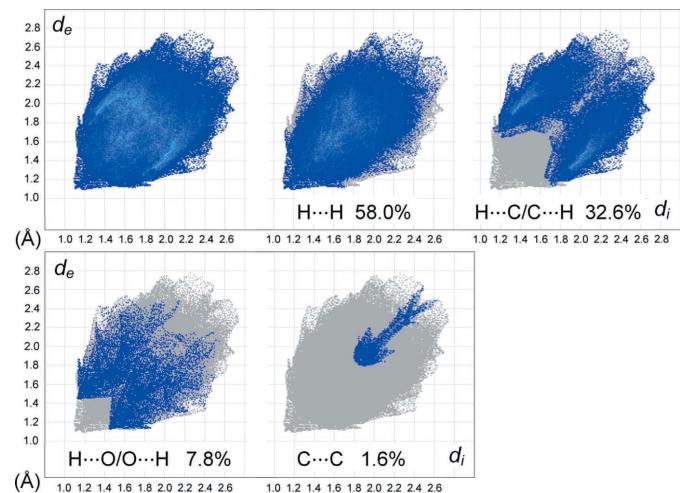
Crystal packing of the title compound, viewed down the b axis, showing how the $\text{C}-\text{H}\cdots\text{O}$ bonded chains (which are orthogonal to the drawing plane) are connected into layers by means of $\text{C}-\text{H}\cdots\pi$ and slipped $\pi-\pi$ stacking interactions. The blue and grey colours indicate two separate bilayers, which lie parallel to the bc plane. [Symmetry codes: (iv) $x, -y + 1, z + \frac{1}{2}$; (v) $-x, -y + 1, -z$.]

4. Database Survey

In the Cambridge Structure Database (CSD, version 5.42, last update November 2020; Groom *et al.*, 2016), no organoantimony tellurates have been deposited, while only five hits are found for other kinds of organometallic TeO_6 -containing compounds. These include the already mentioned organotin derivatives *trans*- $[(\text{Ph}_3\text{SnO})_4\text{Te}(\text{OH})_2]$ and *trans*- $[(\text{Ph}_3\text{SnO})_2\text{Te}(\text{OMe})_4]$ (refcodes: LUWHUH and LUWJAP, Herntrich & Merzweiler, 2010), *trans*- $(\text{Bu}_3\text{SnO})_2[\text{CH}_2(\text{Ph}_2\text{SnO})_2]_2\text{Te}$ (refcode: MOGDER, Beckmann *et al.*, 2002) and two silyloxy compounds bis(μ_2 -oxo)-octakis(trimethylsilyloxy)ditellurium and orthotelluric acid tris(1,1,2,2-tetramethyldisilane-1,2-diyl)ester (refcodes: FAQVUO and FAQWAV, Driess *et al.*, 1999). The sixth known structure, $(\text{Bu}_3\text{SnO})_3\text{Te}(\text{OH})_3$, (Beckmann *et al.*, 2002) is not deposited in the CSD. All of the above compounds feature sixfold O_6 octahedral coordination of the Te atoms, with just one example of a condensed ditellurate core in $(\text{RO})_4\text{Te}(\mu\text{-O})_2\text{Te}(\text{OR})_4$ ($\text{R} = \text{Me}_3\text{Si}$; FAQVUO). The latter contains double Te—O—Te bridges, which are formally similar to the double Te—O—Sb bridges found in the title compound. No tetrahedral TeO_4 fragments have been reported in organometallic series to date. The only known example of a tetrahedral tellurate is the ionic salt $[\text{NEt}_4]_2\text{TeO}_4\cdot 2\text{H}_2\text{O}$ (Konaka *et al.*, 2008).

5. Hirshfeld analysis

Supramolecular interactions in the title structure were further accessed and visualized by Hirshfeld surface analysis (Spackman & Byrom, 1997; McKinnon *et al.*, 2004; Hirshfeld, 1977; Spackman & McKinnon, 2002) performed using *CrystalExplorer17* (Turner *et al.*, 2017). The two-dimensional fingerprint plots (Fig. 5) suggest that the major contributors to

**Figure 5**

The overall two-dimensional fingerprint plot for the title compound, and those delineated into $\text{H}\cdots\text{H}$ (58.0%), $\text{H}\cdots\text{C/C}\cdots\text{H}$ (32.6%), $\text{H}\cdots\text{O}/\text{O}\cdots\text{H}$ (7.8%) and $\text{C}\cdots\text{C}$ (1.6%) contacts.

the Hirshfeld surface are $\text{H}\cdots\text{H}$ (58.0%) and $\text{H}\cdots\text{C/C}\cdots\text{H}$ (32.6%) contacts, while the $\text{H}\cdots\text{O}/\text{O}\cdots\text{H}$ contacts contribute only 7.8%. The latter are identified by a pair of short and very diffuse spikes, at *ca* 2.6 Å, which are actually superimposed upon the regions for the $\text{H}\cdots\text{C/C}\cdots\text{H}$ interactions (the shortest of which is *ca* 2.9 Å). These results are consistent with the weakness of the $\text{C}-\text{H}\cdots\text{O}$ bonds in the structure. It is evident that only a few of the $\text{H}\cdots\text{C/C}\cdots\text{H}$ contacts correspond to $\text{C}-\text{H}\cdots\pi$ bonding. Therefore, the $\text{H}\cdots\text{C/C}\cdots\text{H}$ plot represents a rather diffuse collection of points between the pair of poorly resolved features and there no ‘wings’ at the upper left and lower right, which are characteristic of $\text{C}-\text{H}\cdots\pi$ interactions (Spackman & McKinnon, 2002). The fraction of $\text{C}\cdots\text{C}$ contacts is particularly low (1.6%), indicating only very minor significance of the stacking interactions. In fact, with the exception of the one $\pi-\pi$ stack noted above, this kind of interaction is irrelevant to the title structure.

6. Synthesis and crystallization

In previously reported syntheses, a range of silver salts were used in ion-exchange reactions to form Ph_3SbCl_2 (Goel *et al.*, 1969) and Ph_4SbBr (Goel, 1969) derivatives cleanly and in high yields. Our attempts to prepare tellurate(VI) analogues of such compounds led to dearylation and the formation of mixtures. The title compound was prepared in low yield by reacting the silver salt, $\text{Ag}_3\text{H}_3\text{TeO}_6$, with tetraphenylantimony(V) bromide as follows:

The starting material, $\text{Ag}_3\text{H}_3\text{TeO}_6$, was synthesized according to the method of Gospodinov (1992). 0.220 g (0.4 mmol) of $\text{Ag}_3\text{H}_3\text{TeO}_6$ were added to a solution containing 0.612 g (1.2 mmol) of Ph_4SbBr in 20 mL of acetonitrile. The mixture was stirred for 3 h and then the AgBr precipitate removed by filtration. Evaporation of the solution yielded a colourless glassy material, which was then dissolved in 10 mL

Table 3
Experimental details.

Crystal data	
Chemical formula	[Sb ₃ Te(C ₆ H ₅) ₉ O ₆]
<i>M</i> _r	1282.75
Crystal system, space group	Monoclinic, C2/c
Temperature (K)	173
<i>a</i> , <i>b</i> , <i>c</i> (Å)	47.714 (2), 9.1176 (4), 22.9324 (10)
β (°)	104.168 (4)
<i>V</i> (Å ³)	9672.9 (8)
<i>Z</i>	8
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	2.31
Crystal size (mm)	0.28 × 0.22 × 0.21
Data collection	
Diffractometer	Stoe IPDS
Absorption correction	Numerical [X-RED (Stoe & Cie, 2001) and X-SHAPE (Stoe & Cie, 1999)]
<i>T</i> _{min} , <i>T</i> _{max}	0.499, 0.572
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	29796, 10754, 8356
<i>R</i> _{int}	0.053
(sin θ/λ) _{max} (Å ⁻¹)	0.644
Refinement	
<i>R</i> [F^2 > 2σ(F^2)], <i>wR</i> (F^2), <i>S</i>	0.038, 0.096, 0.93
No. of reflections	10754
No. of parameters	577
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	1.00, -1.24

Computer programs: IPDS Software (Stoe & Cie, 2000), SHELXS97 (Sheldrick, 2008), SHELXL2018/1 (Sheldrick, 2015), DIAMOND (Brandenburg, 1999) and WinGX (Farrugia, 2012).

of a 1:1 v/v mixture of benzene and butyl acetate. Slow evaporation of the solution to a volume of 2–3 mL afforded 0.138 g (27%) of the product in the form of long colourless prisms. The crystals were filtered and dried in air. Analysis (%) for C₅₄H₄₅O₆Sb₃Te: Found: C 50.12, H 3.39; Calculated: C 50.56, H 3.54. IR (KBr, cm⁻¹): 454s, 520m, 610s, 692vs, 732vs, 772w, 996w, 1066m, 1434s, 1478m, 1576w, 2824w, 3052m.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All the hydrogen atoms were located in difference-Fourier maps and then refined as riding with C—H = 0.95 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C).

Funding information

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Tris[triphenylantimony(V)]hexa(μ -oxido)tellurium(VI): a molecular complex with six Te—O—Sb bridges

Kostiantyn V. Domasevitch and Ganna A. Senchyk

Computing details

Data collection: *IPDS Software* (Stoe & Cie, 2000); cell refinement: *IPDS Software* (Stoe & Cie, 2000); data reduction: *IPDS Software* (Stoe & Cie, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018/1* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Hexa- μ -oxido-1:2 κ^4 O:O;1:3 κ^4 O:O;1:4 κ^4 O:O-nonaphenyl-2 κ^3 C,3 κ^3 C,4 κ^3 C-triantimony(V)tellurium(VI)

Crystal data

[Sb₃Te(C₆H₅)₉O₆]

$M_r = 1282.75$

Monoclinic, $C2/c$

$a = 47.714$ (2) Å

$b = 9.1176$ (4) Å

$c = 22.9324$ (10) Å

$\beta = 104.168$ (4)°

$V = 9672.9$ (8) Å³

$Z = 8$

$F(000) = 4976$

$D_x = 1.762$ Mg m⁻³

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

Cell parameters from 8000 reflections

$\theta = 2.2\text{--}27.2$ °

$\mu = 2.31$ mm⁻¹

$T = 173$ K

Prism, colorless

0.28 × 0.22 × 0.21 mm

Data collection

Stoe IPDS

 diffractometer

Radiation source: fine-focus sealed tube

φ oscillation scans

Absorption correction: numerical

 [X-RED (Stoe & Cie, 2001) and X-SHAPE
(Stoe & Cie, 1999)]

$T_{\min} = 0.499$, $T_{\max} = 0.572$

29796 measured reflections

10754 independent reflections

8356 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.053$

$\theta_{\max} = 27.2$ °, $\theta_{\min} = 2.2$ °

$h = -61 \rightarrow 61$

$k = -11 \rightarrow 11$

$l = -22 \rightarrow 29$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.096$

$S = 0.93$

10754 reflections

577 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 1.00$ e Å⁻³

$\Delta\rho_{\min} = -1.24$ 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>	$U_{\text{iso}}^*/U_{\text{eq}}$
Te1	0.11716 (2)	0.68140 (3)	0.04796 (2)	0.02091 (7)
Sb1	0.07040 (2)	0.57473 (3)	-0.06047 (2)	0.02250 (7)
Sb2	0.17996 (2)	0.60629 (3)	0.04935 (2)	0.02511 (8)
Sb3	0.11281 (2)	0.81559 (3)	0.16789 (2)	0.02307 (8)
O1	0.10263 (7)	0.7188 (3)	-0.03781 (13)	0.0251 (6)
O2	0.08497 (7)	0.5513 (3)	0.03277 (13)	0.0242 (6)
O3	0.14157 (7)	0.5152 (3)	0.03645 (14)	0.0272 (7)
O4	0.15241 (7)	0.7840 (3)	0.04941 (14)	0.0259 (6)
O5	0.09873 (7)	0.8455 (3)	0.07399 (13)	0.0242 (6)
O6	0.12791 (7)	0.6419 (3)	0.13479 (13)	0.0256 (6)
C1	0.02873 (10)	0.6340 (5)	-0.0526 (2)	0.0283 (9)
C2	0.02482 (13)	0.7519 (6)	-0.0164 (3)	0.0481 (14)
H2	0.040997	0.806533	0.005257	0.058*
C3	-0.00268 (15)	0.7882 (7)	-0.0124 (3)	0.0578 (17)
H3	-0.005373	0.870350	0.011127	0.069*
C4	-0.02669 (13)	0.7065 (7)	-0.0423 (3)	0.0523 (16)
H4	-0.045521	0.731029	-0.038595	0.063*
C5	-0.02249 (12)	0.5895 (7)	-0.0773 (3)	0.0491 (14)
H5	-0.038624	0.533456	-0.098183	0.059*
C6	0.00518 (11)	0.5525 (6)	-0.0826 (2)	0.0392 (12)
H6	0.007804	0.471373	-0.106653	0.047*
C7	0.06772 (10)	0.6452 (5)	-0.15228 (19)	0.0279 (9)
C8	0.04299 (14)	0.7081 (8)	-0.1870 (3)	0.0572 (17)
H8	0.026270	0.718276	-0.171824	0.069*
C9	0.04280 (16)	0.7567 (10)	-0.2448 (3)	0.075 (2)
H9	0.025760	0.799698	-0.269074	0.090*
C10	0.06683 (17)	0.7434 (9)	-0.2672 (3)	0.065 (2)
H10	0.066485	0.775560	-0.306753	0.078*
C11	0.09166 (15)	0.6821 (7)	-0.2310 (3)	0.0541 (16)
H11	0.108536	0.673533	-0.245738	0.065*
C12	0.09213 (13)	0.6338 (7)	-0.1741 (2)	0.0453 (13)
H12	0.109299	0.592438	-0.149739	0.054*
C13	0.07579 (10)	0.3464 (5)	-0.0738 (2)	0.0253 (9)
C14	0.06436 (11)	0.2885 (5)	-0.1306 (2)	0.0332 (11)
H14	0.055396	0.351604	-0.162692	0.040*
C15	0.06591 (12)	0.1384 (5)	-0.1409 (2)	0.0381 (12)
H15	0.057839	0.098566	-0.179658	0.046*
C16	0.07947 (13)	0.0479 (5)	-0.0935 (3)	0.0418 (13)
H16	0.080622	-0.054577	-0.100017	0.050*

C17	0.09124 (13)	0.1054 (5)	-0.0373 (2)	0.0392 (12)
H17	0.100771	0.042865	-0.005505	0.047*
C18	0.08920 (12)	0.2546 (5)	-0.0271 (2)	0.0351 (11)
H18	0.097003	0.293822	0.011831	0.042*
C19	0.19842 (11)	0.3885 (5)	0.0503 (2)	0.0339 (11)
C20	0.17987 (13)	0.2677 (5)	0.0376 (2)	0.0398 (12)
H20	0.159550	0.282526	0.028564	0.048*
C21	0.19088 (16)	0.1249 (7)	0.0382 (3)	0.0596 (18)
H21	0.178264	0.042909	0.029335	0.071*
C22	0.22051 (19)	0.1063 (7)	0.0519 (4)	0.074 (2)
H22	0.228237	0.010132	0.052558	0.089*
C23	0.23914 (15)	0.2243 (8)	0.0646 (3)	0.0610 (19)
H23	0.259449	0.209139	0.073495	0.073*
C24	0.22796 (13)	0.3664 (7)	0.0644 (3)	0.0454 (13)
H24	0.240714	0.447647	0.074062	0.054*
C25	0.19205 (10)	0.7018 (5)	-0.0260 (2)	0.0296 (10)
C26	0.21692 (14)	0.6580 (8)	-0.0415 (3)	0.0564 (17)
H26	0.228689	0.583115	-0.019206	0.068*
C27	0.22468 (14)	0.7237 (9)	-0.0897 (3)	0.0628 (19)
H27	0.242017	0.694453	-0.099821	0.075*
C28	0.20786 (15)	0.8293 (7)	-0.1229 (3)	0.0537 (16)
H28	0.213614	0.875525	-0.155249	0.064*
C29	0.18223 (19)	0.8685 (9)	-0.1089 (3)	0.073 (2)
H29	0.169940	0.939138	-0.132870	0.088*
C30	0.17436 (15)	0.8053 (7)	-0.0601 (3)	0.0571 (17)
H30	0.156880	0.833491	-0.050383	0.068*
C31	0.20271 (10)	0.6711 (6)	0.1384 (2)	0.0324 (10)
C32	0.21543 (12)	0.5654 (7)	0.1800 (2)	0.0436 (13)
H32	0.215506	0.465302	0.168523	0.052*
C33	0.22812 (15)	0.6083 (9)	0.2390 (3)	0.0637 (19)
H33	0.237072	0.537143	0.267874	0.076*
C34	0.22770 (15)	0.7527 (10)	0.2555 (3)	0.071 (2)
H34	0.236135	0.780978	0.295823	0.085*
C35	0.21508 (13)	0.8571 (8)	0.2136 (3)	0.0560 (16)
H35	0.215294	0.957248	0.225207	0.067*
C36	0.20219 (12)	0.8174 (6)	0.1554 (3)	0.0425 (13)
H36	0.193028	0.889105	0.127008	0.051*
C37	0.13421 (11)	0.7432 (5)	0.2576 (2)	0.0302 (10)
C38	0.15596 (16)	0.6418 (7)	0.2671 (3)	0.0572 (18)
H38	0.162176	0.601976	0.234131	0.069*
C39	0.1691 (2)	0.5966 (8)	0.3264 (3)	0.079 (3)
H39	0.183498	0.522309	0.332976	0.095*
C40	0.16135 (16)	0.6588 (8)	0.3746 (3)	0.0568 (17)
H40	0.170279	0.628873	0.414496	0.068*
C41	0.14045 (14)	0.7650 (7)	0.3639 (2)	0.0484 (14)
H41	0.135249	0.810505	0.397014	0.058*
C42	0.12681 (13)	0.8076 (6)	0.3065 (2)	0.0428 (13)
H42	0.112290	0.881184	0.300325	0.051*

C43	0.12967 (10)	1.0318 (5)	0.1727 (2)	0.0273 (9)
C44	0.15430 (12)	1.0674 (5)	0.2163 (3)	0.0393 (12)
H44	0.163334	0.996960	0.245419	0.047*
C45	0.16574 (14)	1.2099 (6)	0.2169 (3)	0.0506 (15)
H45	0.183074	1.235275	0.245520	0.061*
C46	0.15185 (13)	1.3118 (6)	0.1761 (3)	0.0442 (13)
H46	0.160002	1.406821	0.176095	0.053*
C47	0.12629 (14)	1.2793 (5)	0.1352 (2)	0.0421 (13)
H47	0.116082	1.353112	0.109215	0.050*
C48	0.11567 (12)	1.1371 (5)	0.1323 (2)	0.0341 (11)
H48	0.098727	1.111817	0.102554	0.041*
C49	0.06918 (10)	0.8064 (5)	0.1725 (2)	0.0313 (10)
C50	0.04935 (12)	0.9103 (6)	0.1435 (3)	0.0455 (13)
H50	0.055228	0.985429	0.120348	0.055*
C51	0.02094 (13)	0.9043 (8)	0.1483 (3)	0.0571 (17)
H51	0.007406	0.975992	0.128787	0.069*
C52	0.01240 (14)	0.7942 (9)	0.1813 (3)	0.0604 (19)
H52	-0.006883	0.791890	0.185752	0.072*
C53	0.03177 (14)	0.6876 (8)	0.2080 (3)	0.0540 (17)
H53	0.025482	0.608218	0.228399	0.065*
C54	0.06031 (13)	0.6957 (6)	0.2051 (2)	0.0416 (12)
H54	0.073856	0.625189	0.225552	0.050*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Te1	0.02428 (14)	0.01463 (12)	0.02401 (14)	0.00024 (9)	0.00627 (11)	0.00027 (9)
Sb1	0.02552 (14)	0.01608 (13)	0.02517 (15)	0.00021 (10)	0.00482 (11)	0.00089 (10)
Sb2	0.02550 (15)	0.02110 (14)	0.02942 (16)	0.00203 (10)	0.00803 (12)	0.00078 (11)
Sb3	0.02859 (15)	0.01667 (13)	0.02517 (15)	-0.00063 (10)	0.00892 (11)	0.00024 (10)
O1	0.0306 (16)	0.0175 (13)	0.0268 (15)	-0.0019 (12)	0.0061 (12)	0.0028 (12)
O2	0.0329 (16)	0.0194 (14)	0.0204 (14)	-0.0021 (12)	0.0070 (12)	0.0023 (11)
O3	0.0292 (16)	0.0177 (14)	0.0353 (17)	0.0009 (12)	0.0088 (13)	-0.0024 (12)
O4	0.0295 (16)	0.0148 (13)	0.0338 (17)	-0.0025 (12)	0.0084 (13)	-0.0003 (12)
O5	0.0320 (16)	0.0166 (13)	0.0258 (15)	0.0045 (12)	0.0104 (13)	-0.0015 (11)
O6	0.0323 (17)	0.0184 (14)	0.0259 (15)	0.0011 (12)	0.0068 (13)	-0.0033 (12)
C1	0.030 (2)	0.023 (2)	0.032 (2)	0.0038 (18)	0.0075 (19)	0.0069 (18)
C2	0.042 (3)	0.036 (3)	0.069 (4)	0.005 (2)	0.019 (3)	-0.013 (3)
C3	0.054 (4)	0.049 (3)	0.078 (5)	0.017 (3)	0.031 (3)	-0.002 (3)
C4	0.037 (3)	0.065 (4)	0.061 (4)	0.015 (3)	0.023 (3)	0.020 (3)
C5	0.029 (3)	0.068 (4)	0.050 (3)	-0.006 (3)	0.009 (2)	0.008 (3)
C6	0.032 (3)	0.047 (3)	0.038 (3)	-0.006 (2)	0.008 (2)	-0.003 (2)
C7	0.037 (3)	0.026 (2)	0.020 (2)	-0.0048 (18)	0.0071 (18)	0.0057 (17)
C8	0.045 (3)	0.075 (4)	0.048 (3)	0.000 (3)	0.002 (3)	0.030 (3)
C9	0.056 (4)	0.108 (6)	0.051 (4)	-0.005 (4)	-0.003 (3)	0.042 (4)
C10	0.078 (5)	0.076 (5)	0.039 (3)	-0.011 (4)	0.010 (3)	0.023 (3)
C11	0.063 (4)	0.064 (4)	0.043 (3)	-0.006 (3)	0.028 (3)	0.007 (3)
C12	0.049 (3)	0.055 (3)	0.034 (3)	0.007 (3)	0.015 (2)	0.010 (3)

C13	0.030 (2)	0.0191 (19)	0.027 (2)	0.0001 (16)	0.0080 (18)	-0.0004 (17)
C14	0.035 (3)	0.023 (2)	0.039 (3)	0.0023 (19)	0.003 (2)	-0.0012 (19)
C15	0.049 (3)	0.025 (2)	0.037 (3)	-0.001 (2)	0.003 (2)	-0.006 (2)
C16	0.060 (3)	0.017 (2)	0.052 (3)	0.001 (2)	0.020 (3)	-0.003 (2)
C17	0.064 (4)	0.023 (2)	0.031 (3)	0.011 (2)	0.014 (2)	0.0077 (19)
C18	0.050 (3)	0.026 (2)	0.029 (2)	0.006 (2)	0.011 (2)	0.0035 (19)
C19	0.043 (3)	0.025 (2)	0.039 (3)	0.014 (2)	0.020 (2)	0.0072 (19)
C20	0.050 (3)	0.026 (2)	0.047 (3)	0.011 (2)	0.020 (2)	0.006 (2)
C21	0.077 (5)	0.028 (3)	0.081 (5)	0.020 (3)	0.032 (4)	0.008 (3)
C22	0.099 (6)	0.036 (3)	0.102 (6)	0.032 (4)	0.053 (5)	0.025 (4)
C23	0.055 (4)	0.066 (4)	0.072 (4)	0.037 (3)	0.035 (3)	0.022 (4)
C24	0.045 (3)	0.047 (3)	0.048 (3)	0.019 (3)	0.016 (3)	0.006 (3)
C25	0.031 (2)	0.029 (2)	0.031 (2)	-0.0031 (18)	0.0125 (19)	-0.0010 (18)
C26	0.046 (3)	0.075 (4)	0.057 (4)	0.023 (3)	0.030 (3)	0.027 (3)
C27	0.042 (3)	0.097 (5)	0.056 (4)	0.010 (3)	0.024 (3)	0.025 (4)
C28	0.058 (4)	0.064 (4)	0.046 (3)	-0.010 (3)	0.026 (3)	0.007 (3)
C29	0.095 (6)	0.082 (5)	0.054 (4)	0.036 (5)	0.043 (4)	0.034 (4)
C30	0.063 (4)	0.059 (4)	0.058 (4)	0.025 (3)	0.032 (3)	0.024 (3)
C31	0.023 (2)	0.043 (3)	0.028 (2)	-0.0029 (19)	0.0010 (18)	-0.004 (2)
C32	0.041 (3)	0.053 (3)	0.034 (3)	0.010 (2)	0.003 (2)	0.004 (2)
C33	0.058 (4)	0.091 (5)	0.034 (3)	0.020 (4)	-0.005 (3)	0.005 (3)
C34	0.051 (4)	0.105 (6)	0.045 (4)	0.005 (4)	-0.009 (3)	-0.027 (4)
C35	0.039 (3)	0.066 (4)	0.057 (4)	-0.004 (3)	0.000 (3)	-0.023 (3)
C36	0.033 (3)	0.042 (3)	0.051 (3)	-0.006 (2)	0.007 (2)	-0.012 (2)
C37	0.039 (3)	0.027 (2)	0.022 (2)	-0.0041 (19)	0.0024 (19)	0.0011 (17)
C38	0.080 (5)	0.051 (3)	0.029 (3)	0.032 (3)	-0.007 (3)	-0.005 (2)
C39	0.113 (7)	0.065 (5)	0.046 (4)	0.048 (5)	-0.009 (4)	0.000 (3)
C40	0.077 (5)	0.057 (4)	0.032 (3)	0.004 (3)	0.005 (3)	0.010 (3)
C41	0.056 (4)	0.059 (4)	0.030 (3)	0.002 (3)	0.010 (2)	0.000 (3)
C42	0.046 (3)	0.051 (3)	0.033 (3)	0.005 (3)	0.012 (2)	0.000 (2)
C43	0.033 (2)	0.019 (2)	0.032 (2)	-0.0050 (17)	0.0105 (19)	-0.0021 (17)
C44	0.040 (3)	0.025 (2)	0.048 (3)	-0.004 (2)	0.002 (2)	0.003 (2)
C45	0.052 (3)	0.034 (3)	0.056 (4)	-0.013 (2)	-0.006 (3)	0.002 (3)
C46	0.057 (4)	0.029 (3)	0.046 (3)	-0.015 (2)	0.011 (3)	-0.001 (2)
C47	0.071 (4)	0.023 (2)	0.031 (3)	-0.007 (2)	0.010 (2)	0.0050 (19)
C48	0.049 (3)	0.021 (2)	0.032 (2)	-0.001 (2)	0.009 (2)	0.0022 (18)
C49	0.029 (2)	0.032 (2)	0.034 (2)	-0.0050 (18)	0.0103 (19)	-0.0072 (19)
C50	0.040 (3)	0.045 (3)	0.055 (3)	0.009 (2)	0.017 (3)	0.008 (3)
C51	0.037 (3)	0.072 (4)	0.063 (4)	0.010 (3)	0.013 (3)	-0.010 (3)
C52	0.038 (3)	0.103 (6)	0.043 (3)	-0.024 (4)	0.016 (3)	-0.023 (4)
C53	0.046 (3)	0.079 (5)	0.039 (3)	-0.028 (3)	0.013 (3)	-0.001 (3)
C54	0.045 (3)	0.048 (3)	0.033 (3)	-0.009 (2)	0.010 (2)	0.003 (2)

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

Te1—O2	1.904 (3)	C22—C23	1.380 (11)
Te1—O5	1.904 (3)	C22—H22	0.9500
Te1—O4	1.918 (3)	C23—C24	1.401 (8)

Te1—O1	1.949 (3)	C23—H23	0.9500
Te1—O6	1.964 (3)	C24—H24	0.9500
Te1—O3	1.968 (3)	C25—C30	1.376 (7)
Sb1—O1	1.992 (3)	C25—C26	1.378 (8)
Sb1—O2	2.091 (3)	C26—C27	1.386 (9)
Sb1—C1	2.110 (5)	C26—H26	0.9500
Sb1—C13	2.128 (4)	C27—C28	1.361 (9)
Sb1—C7	2.175 (4)	C27—H27	0.9500
Sb2—O3	1.966 (3)	C28—C29	1.385 (10)
Sb2—O4	2.087 (3)	C28—H28	0.9500
Sb2—C25	2.136 (5)	C29—C30	1.390 (9)
Sb2—C31	2.147 (5)	C29—H29	0.9500
Sb2—C19	2.170 (4)	C30—H30	0.9500
Sb3—O6	1.967 (3)	C31—C32	1.387 (7)
Sb3—O5	2.110 (3)	C31—C36	1.392 (7)
Sb3—C49	2.112 (5)	C32—C33	1.397 (8)
Sb3—C43	2.122 (4)	C32—H32	0.9500
Sb3—C37	2.165 (4)	C33—C34	1.371 (11)
C1—C6	1.381 (7)	C33—H33	0.9500
C1—C2	1.399 (7)	C34—C35	1.381 (11)
C2—C3	1.378 (8)	C34—H34	0.9500
C2—H2	0.9500	C35—C36	1.376 (8)
C3—C4	1.398 (10)	C35—H35	0.9500
C3—H3	0.9500	C36—H36	0.9500
C4—C5	1.379 (9)	C37—C38	1.367 (8)
C4—H4	0.9500	C37—C42	1.385 (7)
C5—C6	1.396 (8)	C38—C39	1.412 (8)
C5—H5	0.9500	C38—H38	0.9500
C6—H6	0.9500	C39—C40	1.371 (10)
C7—C8	1.377 (7)	C39—H39	0.9500
C7—C12	1.380 (8)	C40—C41	1.368 (9)
C8—C9	1.396 (9)	C40—H40	0.9500
C8—H8	0.9500	C41—C42	1.374 (8)
C9—C10	1.371 (11)	C41—H41	0.9500
C9—H9	0.9500	C42—H42	0.9500
C10—C11	1.387 (10)	C43—C44	1.383 (7)
C10—H10	0.9500	C43—C48	1.387 (7)
C11—C12	1.371 (8)	C44—C45	1.408 (7)
C11—H11	0.9500	C44—H44	0.9500
C12—H12	0.9500	C45—C46	1.368 (8)
C13—C18	1.386 (6)	C45—H45	0.9500
C13—C14	1.387 (7)	C46—C47	1.377 (8)
C14—C15	1.394 (7)	C46—H46	0.9500
C14—H14	0.9500	C47—C48	1.387 (7)
C15—C16	1.391 (7)	C47—H47	0.9500
C15—H15	0.9500	C48—H48	0.9500
C16—C17	1.377 (8)	C49—C54	1.382 (7)
C16—H16	0.9500	C49—C50	1.388 (7)

C17—C18	1.388 (7)	C50—C51	1.387 (8)
C17—H17	0.9500	C50—H50	0.9500
C18—H18	0.9500	C51—C52	1.379 (10)
C19—C24	1.382 (8)	C51—H51	0.9500
C19—C20	1.398 (8)	C52—C53	1.377 (10)
C20—C21	1.403 (7)	C52—H52	0.9500
C20—H20	0.9500	C53—C54	1.382 (8)
C21—C22	1.381 (11)	C53—H53	0.9500
C21—H21	0.9500	C54—H54	0.9500
O2—Te1—O5	97.67 (13)	C20—C19—Sb2	118.9 (4)
O2—Te1—O4	166.37 (13)	C19—C20—C21	120.8 (6)
O5—Te1—O4	94.67 (13)	C19—C20—H20	119.6
O2—Te1—O1	81.53 (12)	C21—C20—H20	119.6
O5—Te1—O1	95.83 (13)	C22—C21—C20	118.4 (7)
O4—Te1—O1	91.49 (13)	C22—C21—H21	120.8
O2—Te1—O6	94.01 (13)	C20—C21—H21	120.8
O5—Te1—O6	81.51 (12)	C23—C22—C21	121.5 (6)
O4—Te1—O6	93.53 (13)	C23—C22—H22	119.2
O1—Te1—O6	174.49 (13)	C21—C22—H22	119.2
O2—Te1—O3	88.47 (13)	C22—C23—C24	119.7 (6)
O5—Te1—O3	168.81 (13)	C22—C23—H23	120.2
O4—Te1—O3	80.35 (12)	C24—C23—H23	120.2
O1—Te1—O3	94.32 (13)	C19—C24—C23	120.1 (6)
O6—Te1—O3	88.77 (13)	C19—C24—H24	119.9
O1—Sb1—O2	76.01 (12)	C23—C24—H24	119.9
O1—Sb1—C1	119.50 (15)	C30—C25—C26	119.9 (5)
O2—Sb1—C1	91.35 (15)	C30—C25—Sb2	119.3 (4)
O1—Sb1—C13	124.71 (15)	C26—C25—Sb2	120.7 (4)
O2—Sb1—C13	91.45 (14)	C25—C26—C27	119.7 (6)
C1—Sb1—C13	114.34 (17)	C25—C26—H26	120.1
O1—Sb1—C7	85.22 (15)	C27—C26—H26	120.1
O2—Sb1—C7	161.09 (15)	C28—C27—C26	121.1 (6)
C1—Sb1—C7	99.99 (18)	C28—C27—H27	119.5
C13—Sb1—C7	97.49 (17)	C26—C27—H27	119.5
O3—Sb2—O4	76.38 (12)	C27—C28—C29	119.1 (6)
O3—Sb2—C25	118.46 (16)	C27—C28—H28	120.4
O4—Sb2—C25	88.80 (15)	C29—C28—H28	120.4
O3—Sb2—C31	119.67 (17)	C28—C29—C30	120.5 (6)
O4—Sb2—C31	87.58 (16)	C28—C29—H29	119.7
C25—Sb2—C31	118.87 (19)	C30—C29—H29	119.7
O3—Sb2—C19	88.62 (17)	C25—C30—C29	119.6 (6)
O4—Sb2—C19	164.73 (16)	C25—C30—H30	120.2
C25—Sb2—C19	101.04 (18)	C29—C30—H30	120.2
C31—Sb2—C19	97.6 (2)	C32—C31—C36	120.5 (5)
O6—Sb3—O5	76.45 (12)	C32—C31—Sb2	119.8 (4)
O6—Sb3—C49	116.47 (16)	C36—C31—Sb2	119.4 (4)
O5—Sb3—C49	89.13 (16)	C31—C32—C33	119.0 (6)

O6—Sb3—C43	126.74 (16)	C31—C32—H32	120.5
O5—Sb3—C43	87.41 (15)	C33—C32—H32	120.5
C49—Sb3—C43	113.58 (18)	C34—C33—C32	120.2 (6)
O6—Sb3—C37	89.39 (16)	C34—C33—H33	119.9
O5—Sb3—C37	165.43 (16)	C32—C33—H33	119.9
C49—Sb3—C37	100.46 (19)	C33—C34—C35	120.3 (6)
C43—Sb3—C37	98.58 (17)	C33—C34—H34	119.9
Te1—O1—Sb1	102.08 (13)	C35—C34—H34	119.9
Te1—O2—Sb1	100.07 (13)	C36—C35—C34	120.5 (6)
Sb2—O3—Te1	102.41 (13)	C36—C35—H35	119.7
Te1—O4—Sb2	99.85 (12)	C34—C35—H35	119.7
Te1—O5—Sb3	99.33 (13)	C35—C36—C31	119.4 (6)
Te1—O6—Sb3	102.36 (14)	C35—C36—H36	120.3
C6—C1—C2	119.8 (5)	C31—C36—H36	120.3
C6—C1—Sb1	119.3 (4)	C38—C37—C42	119.4 (5)
C2—C1—Sb1	120.8 (4)	C38—C37—Sb3	121.4 (4)
C3—C2—C1	119.4 (6)	C42—C37—Sb3	119.1 (4)
C3—C2—H2	120.3	C37—C38—C39	119.5 (6)
C1—C2—H2	120.3	C37—C38—H38	120.3
C2—C3—C4	121.2 (6)	C39—C38—H38	120.3
C2—C3—H3	119.4	C40—C39—C38	120.8 (6)
C4—C3—H3	119.4	C40—C39—H39	119.6
C5—C4—C3	118.7 (6)	C38—C39—H39	119.6
C5—C4—H4	120.7	C41—C40—C39	118.5 (5)
C3—C4—H4	120.7	C41—C40—H40	120.8
C4—C5—C6	120.8 (5)	C39—C40—H40	120.8
C4—C5—H5	119.6	C40—C41—C42	121.7 (6)
C6—C5—H5	119.6	C40—C41—H41	119.2
C1—C6—C5	119.9 (5)	C42—C41—H41	119.2
C1—C6—H6	120.0	C41—C42—C37	120.0 (5)
C5—C6—H6	120.0	C41—C42—H42	120.0
C8—C7—C12	120.1 (5)	C37—C42—H42	120.0
C8—C7—Sb1	121.5 (4)	C44—C43—C48	120.4 (4)
C12—C7—Sb1	118.3 (4)	C44—C43—Sb3	120.0 (3)
C7—C8—C9	119.2 (6)	C48—C43—Sb3	119.6 (3)
C7—C8—H8	120.4	C43—C44—C45	118.8 (5)
C9—C8—H8	120.4	C43—C44—H44	120.6
C10—C9—C8	121.0 (6)	C45—C44—H44	120.6
C10—C9—H9	119.5	C46—C45—C44	119.9 (5)
C8—C9—H9	119.5	C46—C45—H45	120.1
C9—C10—C11	118.8 (6)	C44—C45—H45	120.1
C9—C10—H10	120.6	C45—C46—C47	121.3 (5)
C11—C10—H10	120.6	C45—C46—H46	119.3
C12—C11—C10	120.8 (6)	C47—C46—H46	119.3
C12—C11—H11	119.6	C46—C47—C48	119.0 (5)
C10—C11—H11	119.6	C46—C47—H47	120.5
C11—C12—C7	120.2 (5)	C48—C47—H47	120.5
C11—C12—H12	119.9	C43—C48—C47	120.3 (5)

C7—C12—H12	119.9	C43—C48—H48	119.8
C18—C13—C14	119.7 (4)	C47—C48—H48	119.8
C18—C13—Sb1	122.0 (3)	C54—C49—C50	119.6 (5)
C14—C13—Sb1	118.3 (3)	C54—C49—Sb3	119.5 (4)
C13—C14—C15	120.6 (4)	C50—C49—Sb3	120.9 (4)
C13—C14—H14	119.7	C51—C50—C49	120.0 (6)
C15—C14—H14	119.7	C51—C50—H50	120.0
C16—C15—C14	118.9 (5)	C49—C50—H50	120.0
C16—C15—H15	120.5	C52—C51—C50	119.9 (6)
C14—C15—H15	120.5	C52—C51—H51	120.1
C17—C16—C15	120.7 (4)	C50—C51—H51	120.1
C17—C16—H16	119.7	C53—C52—C51	120.1 (6)
C15—C16—H16	119.7	C53—C52—H52	120.0
C16—C17—C18	120.1 (5)	C51—C52—H52	120.0
C16—C17—H17	120.0	C52—C53—C54	120.3 (6)
C18—C17—H17	120.0	C52—C53—H53	119.9
C13—C18—C17	120.0 (5)	C54—C53—H53	119.9
C13—C18—H18	120.0	C53—C54—C49	120.0 (6)
C17—C18—H18	120.0	C53—C54—H54	120.0
C24—C19—C20	119.4 (5)	C49—C54—H54	120.0
C24—C19—Sb2	121.6 (4)		
C6—C1—C2—C3	-1.9 (9)	C27—C28—C29—C30	2.7 (12)
Sb1—C1—C2—C3	179.8 (5)	C26—C25—C30—C29	-2.1 (10)
C1—C2—C3—C4	2.1 (10)	Sb2—C25—C30—C29	179.6 (6)
C2—C3—C4—C5	-1.4 (10)	C28—C29—C30—C25	-0.8 (12)
C3—C4—C5—C6	0.5 (9)	C36—C31—C32—C33	-1.0 (9)
C2—C1—C6—C5	1.1 (8)	Sb2—C31—C32—C33	-174.9 (5)
Sb1—C1—C6—C5	179.4 (4)	C31—C32—C33—C34	0.6 (10)
C4—C5—C6—C1	-0.3 (9)	C32—C33—C34—C35	-0.9 (12)
C12—C7—C8—C9	1.5 (10)	C33—C34—C35—C36	1.5 (11)
Sb1—C7—C8—C9	177.5 (6)	C34—C35—C36—C31	-1.9 (10)
C7—C8—C9—C10	-0.4 (12)	C32—C31—C36—C35	1.6 (9)
C8—C9—C10—C11	-0.8 (13)	Sb2—C31—C36—C35	175.5 (5)
C9—C10—C11—C12	0.9 (11)	C42—C37—C38—C39	4.5 (10)
C10—C11—C12—C7	0.3 (10)	Sb3—C37—C38—C39	-179.4 (6)
C8—C7—C12—C11	-1.5 (9)	C37—C38—C39—C40	-3.4 (13)
Sb1—C7—C12—C11	-177.5 (5)	C38—C39—C40—C41	0.4 (13)
C18—C13—C14—C15	0.9 (8)	C39—C40—C41—C42	1.5 (11)
Sb1—C13—C14—C15	-176.5 (4)	C40—C41—C42—C37	-0.4 (10)
C13—C14—C15—C16	-0.9 (8)	C38—C37—C42—C41	-2.7 (9)
C14—C15—C16—C17	-0.1 (9)	Sb3—C37—C42—C41	-178.9 (5)
C15—C16—C17—C18	1.2 (9)	C48—C43—C44—C45	-3.4 (8)
C14—C13—C18—C17	0.2 (8)	Sb3—C43—C44—C45	177.3 (5)
Sb1—C13—C18—C17	177.5 (4)	C43—C44—C45—C46	2.5 (10)
C16—C17—C18—C13	-1.2 (9)	C44—C45—C46—C47	1.7 (10)
C24—C19—C20—C21	-1.1 (8)	C45—C46—C47—C48	-5.0 (10)
Sb2—C19—C20—C21	-179.5 (5)	C44—C43—C48—C47	0.2 (8)

C19—C20—C21—C22	0.4 (10)	Sb3—C43—C48—C47	179.5 (4)
C20—C21—C22—C23	-0.2 (12)	C46—C47—C48—C43	4.0 (9)
C21—C22—C23—C24	0.7 (12)	C54—C49—C50—C51	1.3 (9)
C20—C19—C24—C23	1.5 (9)	Sb3—C49—C50—C51	-178.4 (5)
Sb2—C19—C24—C23	180.0 (4)	C49—C50—C51—C52	-0.7 (10)
C22—C23—C24—C19	-1.4 (10)	C50—C51—C52—C53	-2.1 (10)
C30—C25—C26—C27	3.1 (10)	C51—C52—C53—C54	4.3 (9)
Sb2—C25—C26—C27	-178.6 (6)	C52—C53—C54—C49	-3.7 (9)
C25—C26—C27—C28	-1.2 (12)	C50—C49—C54—C53	0.9 (8)
C26—C27—C28—C29	-1.7 (12)	Sb3—C49—C54—C53	-179.3 (4)

Hydrogen-bond geometry (\AA , $^\circ$)

$D\text{—H}\cdots A$	$D\text{—H}$	$H\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
C16—H16 \cdots O1 ⁱ	0.95	2.58	3.342 (6)	137
C17—H17 \cdots O5 ⁱ	0.95	2.58	3.437 (6)	150
C21—H21 \cdots O4 ⁱ	0.95	2.75	3.651 (8)	158
C46—H46 \cdots O6 ⁱⁱ	0.95	2.67	3.276 (6)	122
C47—H47 \cdots O6 ⁱⁱ	0.95	2.73	3.307 (6)	120
C47—H47 \cdots O2 ⁱⁱ	0.95	2.70	3.645 (6)	177

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$.