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

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In the structure of the title compound [systematic name hexa-μ-oxido-
1:2x2O:O:1:3x2O:O:1:4x2O:O-nonaphenyl-2x3C,3x3C,4x3C-triantimony(V)tellur-
ium(VI)], [Sb3Te(C6H5)9O6], the hexaoxidotellurate(VI) ion is coordinated to
three SbV ions via pairs of cis-positioned O atoms to form a discrete molecular
unit. The TeVI and SbV central ions exhibit distorted octahedral [TeO6]
and distorted trigonal–bipyramidal [SbC3O2] 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···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
dications 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

Organoantimony(V) species readily form covalent derivatives
with a range of organic and inorganic o xo-ions and these can
be used in the construction of metal–oxide clusters (Nicholson
et al., 2011). Unlike the series of molecular fivefold-coordi-
nated tetraphenylantimony(V) compounds, which easily
dissociate in solution to yield tetraphenylstibonium cations,
[Ph4Sb]+ (Domasevitch et al., 2000), the derivatives of tri-
phenylantimony(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 [Ph3Sb]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 [ReO4]− (Wirringa et al., 1992)
or [PhSO4]− (Rüther et al., 1986) groups or bridging
[Ph3PO4]− groups (Srngavruksam & 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-
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 $\text{M}{}^{(\mu-\text{O})}_2\text{Sb}$ 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 hexaoxotellurate(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.

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)° (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) Å, which occurs in the Te1($\mu$-O)2Sb2 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 $[(\text{Ph}_3\text{SnO})_4\text{Te(OH)}_2]$ and $[(\text{Ph}_3\text{SnO})_2\text{Te}{}^{(\mu-\text{Sb})}_3\text{OMe}_4]$ (Herntrich & Merzweiler, 2010).

The Te1 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)°. The fivefold coordination around each of three Sb-atoms can best be described as distorted trigonal bipyramidal, with the O2—Sb1—C7 = 161.09 (15)°, O4—Sb2—C19 = 164.73 (16)° and O5—Sb3—C37 = 165.43 (16)° bond angles defining the principal axes of the trigonal bipyramids. This assignment is supported by the calculated five-coordinate $\tau$-indices, which are $0.69$, $0.75$ and $0.65$ for Sb1, Sb2 and Sb3, respectively.

Table 1

| Te1—O2 | 1.90 (3) | Sb2—O3 | 1.96 (3) |
| Te1—O5 | 1.90 (3) | Sb2—O4 | 2.08 (3) |
| Te1—O1 | 1.94 (3) | Sb2—C25 | 2.13 (5) |
| Te1—O6 | 1.96 (4) | Sb2—C19 | 2.17 (4) |
| Te1—O3 | 1.98 (3) | Sb3—O3 | 1.97 (3) |
| Sb1—O1 | 1.92 (3) | Sb3—O5 | 2.11 (3) |
| Sb1—O2 | 2.09 (3) | Sb3—C49 | 2.11 (5) |
| Sb1—C1 | 2.11 (5) | Sb3—C3 | 2.12 (4) |
| Sb1—C3 | 2.12 (4) | Sb3—C37 | 2.16 (5) |
| Sb1—C7 | 2.17 (4) |

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.
configuration (Fig. 2). This is consistent with the substituted tellurates, e.g. mer-[Bu₃SnO)₃Te(OH)₃] (Beckmann et al., 2002).

In each of the three Sb-based trigonal bipyramids, the axial Sb—O₆ 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—O6 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—O₆, lie in the range 1.904 (3)–1.966 (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—O₆Sb and Te—O₆Sb 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 polynaphthyl substituted species, e.g. 1,3,5,7-tetraphenyladamantane, supporting a complex framework of aromatic 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⋯O6 = 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⋯π and C41—H41⋯π (where Cg is a ring centroid; symmetry codes: (i) x, y – 1, z; (ii) x, y + 2, x – 1/2; (iv) x, –y + 1, z + 1/2), with C⋯π separations of 3.775 (6) and 3.505 (6) Å 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) = 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.

### Table 2

| C—H⋯A    | D—H | H⋯A | D⋯A | D—H⋯A |
|----------|-----|-----|-----|-------|
| C16—H16⋯O1' | 0.95 | 2.58 | 3.342 (6) | 137 |
| C17—H17⋯O5' | 0.95 | 2.58 | 3.437 (6) | 150 |
| C21—H21⋯O4' | 0.95 | 2.75 | 3.651 (8) | 158 |
| C46—H46⋯O6' | 0.95 | 2.67 | 3.276 (6) | 122 |
| C47—H47⋯O6" | 0.95 | 2.73 | 3.367 (6) | 120 |
| C47—H47⋯O2" | 0.95 | 2.70 | 3.645 (6) | 177 |

Symmetry codes: (i) x, y – 1, z; (ii) x, y + 1, z.
derivatives trans compounds. These include the already mentioned organotin et al. (refcode: MOGDER, Beckmann fingerprint plots (Fig. 5) suggest that the major contributors to talExplorer17 (Turner 1977; Spackman & McKinnon, 2002) performed using Crys-
[NEt4]2TeO4 known example of a tetrahedral tellurate is the ionic salt have been reported in organometallic series to date. The only +
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 + 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 organoantimon- mony tellurates have been deposited, while only five hits are found for other kinds of organometallic TeO6-containing compounds. These include the already mentioned organotin derivatives trans-[{Ph(SnO)2}2Te(OH)2] and trans-[{Ph(SnO)2}2Te(OMe)2] (refcodes: LUWHUH and LUWJAP, Herntreich & Merzweiler, 2010), trans-(Bu3SnO)2[CH2(Ph3SnO)2]2Te (refcode: MOGDER, Beckmann et al., 2002) and two siloxy compounds bis(µ-oxo)-octakis(trimethylsilyloxy)ditellurium and orthotelluric acid tris(1,1,2,2-tetramethylsilisilane-1,2-diy)-ester (refcodes: FAQVUO and FAQWAV, Driess et al., 1999). The sixth known structure, (Bu3SnO)2Te(OH)2, (Beckmann et al., 2002) is not deposited in the CSD. All of the above compounds feature sixfold O6 octahedral coordination of the Te atoms, with just one example of a condensed ditellurate core in (RO)4Te(µ-O)2Te(OR)4 (R = Me3Si; 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 TeO4 fragments have been reported in organometallic series to date. The only known example of a tetrahedral tellurate is the ionic salt [NEt4]2TeO4-2H2O (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 the Hirshfeld surface are H···H (58.0%) and H···C/C···H (32.6%) contacts, while the H···O/O···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 H···C/C···H interactions (the shortest of which is ca 2.9 Å). These results are consistent with the weakness of the C—H···O bonds in the structure. It is evident that only a few of the H···C/C···H contacts correspond to C—H···π bonding. Therefore, the H···C/C···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 C—
H···π interactions (Spackman & McKinnon, 2002). The fraction of C···C contacts is particularly low (1.6%), indicating only very minor significance of the stacking interactions. In fact, with the exception of the one π···π 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 Ph3SbCl2 (Goel et al., 1969) and Ph3SbBr (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, Ag2H2TeO6, with tetraphenylantimony(V) bromide as follows:

The starting material, Ag2H2TeO6, was synthesized according to the method of Gospodinov (1992). 0.220 g (0.4 mmol) of Ag2H2TeO6 were added to a solution containing 0.612 g (1.2 mmol) of Ph3SbBr 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

Figure 4
Crystal packing of the title compound, viewed down the b axis, showing how the C—H···O bonded chains (which are orthogonal to the drawing plane) are connected into layers by means of C—H···π and slipped π···π 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 + 1/2; (v) −x, −y + 1, −z.]

Figure 5
The overall two-dimensional fingerprint plot for the title compound, and those delineated into H···H (58.0%), H···C/C···H (32.6%), H···O/O···H (7.8%) and C···C (1.6%) contacts.
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 (1): 454 m, 2824 s, 1576 m, 1434 s, 1478 m, 8356 w, 732 vs, 610 m, 506 vs. vs, 305 vs. vs, 200 km. h = 0.95 Å and $U_{eq}(H) = 1.2U_{eq}(C)$.

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 $U_{eq}(H) = 1.2U_{eq}(C)$.

Funding information
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Table 3
Experimental details.

| Crystal data | Chemical formula | [Sb$_3$Te(C$_6$H$_5$)$_9$O$_6$] |
|--------------|------------------|-------------------------------|
| $M_r$        | 1262.75          |
| Crystal system, space group | Monoclinic, C2/c |
| Temperature (K) | 173 |
| $a$, $b$, $c$ (Å) | 47.714 (2), 9.1176 (4), 22.9324 (10) |
| $\beta$ (°) | 104.168 (4) |
| $V$ (Å$^3$) | 9672.9 (8) |
| $Z$ | 8 |
| Radiation type | Mo Kα |
| $\mu$ (mm$^{-1}$) | 2.31 |
| Crystal size (mm) | 0.28 × 0.22 × 0.21 |

Data collection
| Absorption correction | Numerical [X-RED (Stoe & Cie, 2001) and X-SHAPE (Stoe & Cie, 1999)] |
| $T_{min}$, $T_{max}$ | 0.490, 0.572 |
| No. of measured, independent and observed | 29796, 10754, 8356 |
| $R_{int}$ | 0.053 |
| $\langle \sin \theta/\lambda \rangle_{max}$ (Å$^{-1}$) | 0.644 |

Refinement
| $R(F^2 > 2\sigma(F^2))$, $wR(F^2)$, $S$ | 0.038, 0.096, 0.93 |
| No. of reflections | 10754 |
| No. of parameters | 577 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta \rho_{max}$, $\Delta \rho_{min}$ (e Å$^{-3}$) | 1.00, –1.24 |

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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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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-1:2κ⁴O;O;1:3κ⁴O;O;1:4κ⁴O;O-nonaphenyl-2κ⁴C,3κ⁴C,4κ⁴C-triantimony(V)tellurium(VI)

Crystal data

[Sb₃Te(C₆H₅)₉O₆]  \( F(000) = 4976 \)

\( M_r = 1282.75 \)

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

\( Z = 8 \)

Data collection

Stoe IPDS
diffractometer

Radiation source: fine-focus sealed tube

\( \varphi \) oscillation scans

Absorption correction: numerical

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

\( T_{\text{min}} = 0.499, T_{\text{max}} = 0.572 \)

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

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

where \( P = (F_c^2 + 2F_s^2)/3 \)

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

\( \Delta\rho_{\text{max}} = 1.00 \) e Å⁻³

\( \Delta\rho_{\text{min}} = -1.24 \) 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 (Å²)

| x     | y     | z     | U_iso*/U_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) |
| C5    | −0.045521 | 0.731029 | −0.038595 | 0.063* |
| H5    | −0.038624 | 0.533456 | −0.098183 | 0.059* |
| C6    | 0.00518 (11) | 0.5525 (6) | −0.0826 (2) | 0.0392 (12) |
| C7    | 0.007804 | 0.471373 | −0.106653 | 0.047* |
| C8    | 0.06772 (10) | 0.6452 (5) | −0.15228 (19) | 0.0279 (9) |
| C9    | 0.04299 (14) | 0.7081 (8) | −0.1870 (3) | 0.0572 (17) |
| C10   | 0.025760 | 0.799698 | −0.269074 | 0.090* |
| C11   | 0.066830 (17) | 0.7434 (9) | −0.2672 (3) | 0.065 (2) |
| C12   | 0.066485 | 0.775560 | −0.306753 | 0.078* |
| C13   | 0.09166 (15) | 0.6821 (7) | −0.2310 (3) | 0.0541 (16) |
| C14   | 0.108536 | 0.673533 | −0.245738 | 0.065* |
| C15   | 0.09213 (13) | 0.6338 (7) | −0.1741 (2) | 0.0453 (13) |
| C16   | 0.109299 | 0.592438 | −0.149739 | 0.054* |
| C17   | 0.07579 (10) | 0.3464 (5) | −0.0738 (2) | 0.0253 (9) |
| C18   | 0.06436 (11) | 0.2885 (5) | −0.1306 (2) | 0.0332 (11) |
| C19   | 0.055396 | 0.351604 | −0.162692 | 0.040* |
| C20   | 0.06591 (12) | 0.1384 (5) | −0.1409 (2) | 0.0381 (12) |
| C21   | 0.057839 | 0.098566 | −0.179658 | 0.046* |
| C22   | 0.07947 (13) | 0.0479 (5) | −0.0935 (3) | 0.0418 (13) |
| C23   | 0.080622 | −0.054577 | −0.100017 | 0.050* |
| Atom | x       | y       | z       | U11 | U22 | U33 | U12 | U13 | U23 | U31 | U32 | U31 | U32 | U31 | U32 | U31 | U32 | U31 | U32 | U31 | U32 |
|------|---------|---------|---------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| C17  | 0.09124 | 0.1054  | −0.0373 | 0.0392 | 0.047* |
| H17  | 0.10077 | 0.042865| −0.005505| 0.0351 | 0.042* |
| C18  | 0.08920 | 0.2546  | −0.0271 | 0.0392 | 0.0339 |
| H18  | 0.097003| 0.293822| 0.011831| 0.0398 | 0.048* |
| C19  | 0.19842 | 0.3885  | 0.0503  | 0.0398 | 0.0596 |
| H20  | 0.15955 | 0.28256 | 0.028564| 0.0596 | 0.071* |
| C21  | 0.19088 | 0.1249  | 0.0382  | 0.0596 | 0.074 (2) |
| H22  | 0.22051 | 0.1063  | 0.0519  | 0.0610 | 0.089* |
| C23  | 0.23914 | 0.2243  | 0.0646  | 0.0610 | 0.089* |
| H24  | 0.259449| 0.209139| 0.073495| 0.073* | 0.073* |
| C25  | 0.22796 | 0.3664  | 0.0644  | 0.075 (3) |
| C26  | 0.240714| 0.447647| 0.074062| 0.075 (3) |
| C27  | 0.19205 | 0.7018  | −0.0260 | 0.0564 | 0.0928 |
| C28  | 0.21692 | 0.6580  | −0.0415 | 0.0564 | 0.106 (3) |
| C29  | 0.228689| 0.583115| −0.019206| 0.068* | 0.106 (3) |
| C30  | 0.22468 | 0.7237  | −0.0897 | 0.068* | 0.106 (3) |
| C31  | 0.242017| 0.694453| −0.099821| 0.075 (3) |
| C32  | 0.20786 | 0.8293  | −0.1229 | 0.075 (3) |
| C33  | 0.213614| 0.875525| −0.155249| 0.075 (3) |
| C34  | 0.18223 | 0.8685  | −0.1089 | 0.075 (3) |
| C35  | 0.169940| 0.939138| −0.132870| 0.088* |
| C36  | 0.17436 | 0.8053  | −0.0601 | 0.088* | 0.106 (3) |
| C37  | 0.156880| 0.833491| −0.050383| 0.088* |
| C38  | 0.20271 | 0.6711  | 0.1384  | 0.088* | 0.106 (3) |
| C39  | 0.21543 | 0.5654  | 0.1800  | 0.088* | 0.106 (3) |
| C40  | 0.215506| 0.465302| 0.168523| 0.088* | 0.106 (3) |
| C41  | 0.22812 | 0.6083  | 0.2390  | 0.088* | 0.106 (3) |
| C42  | 0.237072| 0.537143| 0.267874| 0.088* | 0.106 (3) |
| C43  | 0.22770 | 0.7527  | 0.2555  | 0.088* | 0.106 (3) |
| C44  | 0.236135| 0.780978| 0.295823| 0.088* | 0.106 (3) |
| C45  | 0.21508 | 0.8571  | 0.2136  | 0.088* | 0.106 (3) |
| C46  | 0.215294| 0.957248| 0.225207| 0.088* | 0.106 (3) |
| C47  | 0.20219 | 0.8174  | 0.1554  | 0.088* | 0.106 (3) |
| C48  | 0.193028| 0.889105| 0.127008| 0.088* | 0.106 (3) |
| C49  | 0.13421 | 0.7432  | 0.2576  | 0.088* | 0.106 (3) |
| C50  | 0.15596 | 0.6418  | 0.2671  | 0.088* | 0.106 (3) |
| C51  | 0.162176| 0.601976| 0.234131| 0.088* | 0.106 (3) |
| C52  | 0.1691 | 0.5966  | 0.3264  | 0.088* | 0.106 (3) |
| C53  | 0.183498| 0.522309| 0.332976| 0.088* | 0.106 (3) |
| C54  | 0.16135 | 0.6588  | 0.3746  | 0.088* | 0.106 (3) |
| C55  | 0.170279| 0.628873| 0.414496| 0.088* | 0.106 (3) |
| C56  | 0.14045 | 0.7650  | 0.3639  | 0.088* | 0.106 (3) |
| C57  | 0.135249| 0.810505| 0.397014| 0.088* | 0.106 (3) |
| C58  | 0.12681 | 0.8076  | 0.3065  | 0.088* | 0.106 (3) |
| C59  | 0.112290| 0.881184| 0.300325| 0.088* | 0.106 (3) |
### Atomic displacement parameters (Å²)

|     | $U^{11}$  | $U^{22}$  | $U^{33}$  | $U^{12}$  | $U^{13}$  | $U^{23}$  |
|-----|-----------|-----------|-----------|-----------|-----------|-----------|
| 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)   |
### Geometric parameters (Å, °)

|            |          |              |                |                |                 |                 |
|------------|----------|--------------|----------------|----------------|-----------------|-----------------|
| 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)      |                |                 |                 |

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) −0.002 (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) 0.005 (19)
C48 0.049 (3) 0.021 (2) 0.032 (2) −0.001 (2) 0.009 (2) 0.002 (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)
| Bond | Distance (Å) | Bond | Distance (Å) |
|------|-------------|------|-------------|
| 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) |
| Bond | Distance (Å) |
|------|-------------|
| C17—C18 | 1.388 (7) |
| C17—H17 | 0.9500 |
| C18—H18 | 0.9500 |
| C19—C24 | 1.382 (8) |
| C19—C20 | 1.398 (8) |
| C20—C21 | 1.403 (7) |
| C20—H20 | 0.9500 |
| C21—C22 | 1.381 (11) |
| C21—H21 | 0.9500 |
| C22—C23 | 1.381 (11) |
| C22—H22 | 0.9500 |
| C23—C24 | 1.382 (8) |
| C23—H23 | 0.9500 |
| C24—C25 | 1.387 (8) |
| C24—H24 | 0.9500 |
| O2—Te1—O5 | 97.67 (13) |
| O2—Te1—O4 | 166.37 (13) |
| O2—Te1—O1 | 81.53 (12) |
| O5—Te1—O4 | 95.83 (13) |
| O4—Te1—O1 | 91.49 (13) |
| O2—Te1—O6 | 94.01 (13) |
| O5—Te1—O6 | 81.51 (12) |
| O4—Te1—O6 | 93.53 (13) |
| O1—Te1—O6 | 174.49 (13) |
| O2—Te1—O3 | 88.47 (13) |
| O5—Te1—O3 | 168.81 (13) |
| O4—Te1—O3 | 80.35 (12) |
| O1—Te1—O3 | 94.32 (13) |
| O6—Te1—O3 | 88.77 (13) |
| O1—Sb1—O2 | 76.01 (12) |
| O1—Sb1—C1 | 119.50 (15) |
| O2—Sb1—C1 | 91.35 (15) |
| O1—Sb1—C13 | 124.71 (15) |
| O2—Sb1—C13 | 91.45 (14) |
| C1—Sb1—C13 | 114.34 (17) |
| O1—Sb1—C7 | 85.22 (15) |
| O2—Sb1—C7 | 161.09 (15) |
| C1—Sb1—C7 | 99.99 (18) |
| C13—Sb1—C7 | 97.49 (17) |
| O3—Sb2—O4 | 76.38 (12) |
| O3—Sb2—C25 | 118.46 (16) |
| O4—Sb2—C25 | 88.80 (15) |
| O3—Sb2—C31 | 119.67 (17) |
| O4—Sb2—C31 | 87.58 (16) |
| C25—Sb2—C31 | 118.87 (19) |
| O3—Sb2—C19 | 88.62 (17) |
| O4—Sb2—C19 | 164.73 (16) |
| C25—Sb2—C19 | 101.04 (18) |
| C31—Sb2—C19 | 97.6 (2) |
| O6—Sb3—O5 | 76.45 (12) |
| O6—Sb3—C49 | 116.47 (16) |
| O5—Sb3—C49 | 89.13 (16) |
| Bond                  | Angle (deg) (E) | Bond                  | Angle (deg) (E) |
|----------------------|----------------|----------------------|----------------|
| 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)    | C35—C34—C36         | 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  179.8 (5)  C27—C28—C29—C30  2.7 (12)
Sb1—C1—C2—C3  1.9 (9)  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)  \quad \text{Sb3—C43—C48—C47}  179.5 (4)
C20—C21—C22—C23 −0.2 (12)  \quad \text{C46—C47—C48—C43}  4.0 (9)
C21—C22—C23—C24  0.7 (12)  \quad \text{C54—C49—C50—C51}  1.3 (9)
C20—C19—C24—C23  1.5 (9)  \quad \text{Sb3—C49—C50—C51}  −178.4 (5)
Sb2—C19—C24—C23  180.0 (4)  \quad \text{C49—C50—C51—C52}  −0.7 (10)
C22—C23—C24—C19 −1.4 (10)  \quad \text{C50—C51—C52—C53}  −2.1 (10)
C30—C25—C26—C27  3.1 (10)  \quad \text{C51—C52—C53—C54}  4.3 (9)
Sb2—C25—C26—C27 −178.6 (6)  \quad \text{C52—C53—C54—C49}  −3.7 (9)
C25—C26—C27—C28 −1.2 (12)  \quad \text{C50—C49—C54—C53}  0.9 (8)
C26—C27—C28—C29 −1.7 (12)  \quad \text{Sb3—C49—C54—C53}  −179.3 (4)

*Hydrogen-bond geometry (Å, °)*

| D—H···A   | D—H  | H···A   | D···A     | D—H···A |
|-----------|-------|---------|-----------|---------|
| C16—H16···O1i  | 0.95  | 2.58    | 3.342 (6) | 137     |
| C17—H17···O5i  | 0.95  | 2.58    | 3.437 (6) | 150     |
| C21—H21···O4i  | 0.95  | 2.75    | 3.651 (8) | 158     |
| C46—H46···O6ii | 0.95  | 2.67    | 3.276 (6) | 122     |
| C47—H47···O6ii | 0.95  | 2.73    | 3.307 (6) | 120     |
| C47—H47···O2ii | 0.95  | 2.70    | 3.645 (6) | 177     |

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