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# [$\mu_2$-2,5-Dimercapto-1,3,4-thiadiazole(2–)-$\kappa^2N$:$N$]bis($\mu_2$-methanolato)-$\mu_3$-oxido-tris[bis(4-fluorobenzyl)tin(IV)] benzene hemisolvate

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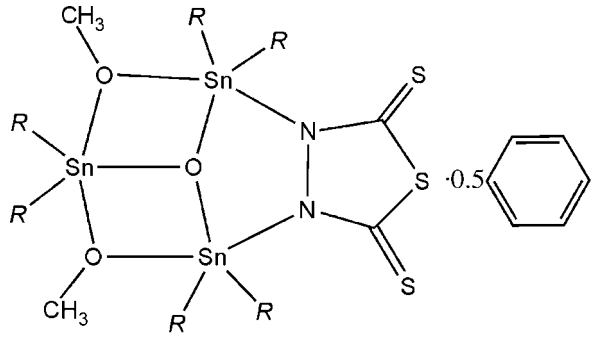
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.016 Å; $R$ factor = 0.055; $wR$ factor = 0.184; data-to-parameter ratio = 16.6.

The title complex, $[Sn_3(C_7H_7F)_6(CH_3O)_2(C_2N_2S_3)O]\cdot0.5C_6H_6$, contains a unique $\mu_3$-$OSn_3N_2O_2$ central core with three five-coordinated Sn atoms with distorted trigonal–bipyramidal geometries; the benzene molecule resides on a crystallographic inversion center (at the ring centroid). One Sn atom (with a $C_2O_3$ ligand set) has Sn—O bond lengths in the range 2.044 (4)–2.131 (5) Å; the remaining two Sn atoms (with $C_2O_2N$ ligand sets) have Sn—O distances ranging from 2.038 (5) to 2.188 (5) Å. The two Sn—N bond lengths are 2.217 (5) and 2.225 (6) Å, and the six Sn—C bond lengths range from 2.125 (8) to 2.150 (8) Å. There are no clasical hydrogen bonds in the crystal structure.

## Related literature

For related literature, see: ladder-type $Sn_3O_3$ arrangements (Puff *et al.*, 1983), trinuclear *R*SnO clusters (Ma *et al.*, 2007), a staircase $Sn_4O_{10}$ structure (Yin *et al.*, 2006), related Sn ladder systems (Harrison *et al.*, 1980), and van der Waals radii of Sn and N atoms (Hubeey *et al.*, 1993).




$R$ = 4-F-$C_6H_4CH_2$

## Experimental

### Crystal data

$[Sn_3(C_7H_7F)_6(CH_3O)_2(C_2N_2S_3)O]\cdot0.5C_6H_6$
$M_r$ = 1276.12
Monoclinic, $P2_1/c$
$a$ = 10.3309 (9) Å
$b$ = 45.937 (4) Å
$c$ = 13.5763 (8) Å
$\beta$ = 129.394 (4)°
$V$ = 4979.1 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.68 mm$^{-1}$
$T$ = 293 (2) K
0.18 × 0.16 × 0.08 mm

### Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.751, $T_{max}$ = 0.877
51752 measured reflections
9782 independent reflections
8279 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.184
$S$ = 1.01
9782 reflections
591 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.72 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.78 e Å$^{-3}$

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2020).

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# supplementary materials

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# [$\mu_2$-2,5-Dimercapto-1,3,4-thiadiazole(2-)-$\kappa^2N$:$N$]bis($\mu_2$-methanolato)-$\mu_3$-oxido-tris[bis(4-fluorobenzyl)tin(IV)] benzene hemisolvate

**J.-H. Zhang, C.-L. Ma and R.-F. Zhang**

## Comment

From Fig. 1, like other trinuclear organotin-$\mu_3$oxo clusters (Ma *et al.*, 2007), the complex (I) contains a tricyclic system formed from a $N_2Sn_2O$ ring and two $Sn_2O_2$ rings: all three Sn atoms exhibit severely distorted trigonal bipyramidal configurations. The atoms Sn2 and Sn3 have similar environments, in which one O atom and two C atoms of the benzyl groups occupy the equatorial positions (C5, C12 and O1 for Sn2; C19, C26 and O1 for Sn3). The axial positions are occupied by one N atom of the HHdmt and one O atom of the methoxy group (N2 and O2 for Sn1; N1 and O3 for Sn3). The geometry of Sn1 is *cis*-$R_2SnO_3$, in which the axial positions are defined by O2 and O3 atoms of methoxy group, C33 and C40 atoms of benzyl groups and one O atom occupy the equatorial plane.

With regard to the role of reaction hydrolysis, three $[(C_7H_7F)_2Sn]$ units are bridged by one O atom and two O atoms of methoxy group, forming a trinuclear complex, containing two $Sn_2O_2$ rings. Three Sn atoms and three O atoms (Sn1, Sn2, Sn3, O1, O2, O3) comprise a fused ring system, which is similar to traditional hydrolytic products of ladder-type arrangement (Puff *et al.*, 1983), but different from the staircase structure of $C_{84}H_{148}N_8O_{10}Sn_4$ (Yin *et al.*, 2006). The Sn—O distances lies in the range 2.038 (5) to 2.188 (5) Å (Table 1), which are consistent with those Sn—O bonds in the ladder structure reported (Harrison *et al.*, 1980). All of above indicates that strong bridge-oxo coordination with Sn atoms exist in the complex. Moreover, the aromatic rings effectively surround the –O—$CH_3$ group.

The HHdmt ligand forms a five-membered ring, where two N atoms bond to the two Sn atoms to form another five-membered $N_2Sn_2O_1$ ring. The Sn—N bond lengths [Sn2—N2 2.225 (6) Å and Sn3—N1 2.217 (7) Å] approach the covalent radii of Sn and N (2.15 Å) and are much shorter than the van der Waal's radii of Sn and N atoms (3.74 Å) (Hubeey *et al.*, 1993), proving that N is coordinated to Sn by strong chemical bonds.

## Experimental

The 2,5-dimercapto-1,3,4-thiadiazole (1 mmol) was added to the solution of methanol 20 ml with sodium methoxide (2 mmol), and the mixture was stirred for 30 minutes, then di(4-fluorobenzyl)tin (3 mmol) was added to the mixture, continuing the reaction for 12 h at 318k. After cooling down to room temperature, this was then filtered. The solvent of the filtrate was gradually removed by evaporation under vacuum until a solid product was obtained. The solid was then recrystallized from benzene and colorless crystals suitable for X-ray diffraction was obtained (m.p. 356 K). Analysis, calculated for $C_{49}H_{15}F_6N_2O_3S_3Sn_3$: C 46.11, H 3.55, N 2.20; found: C 46.16, H 3.59, N 2.18%.

## Refinement

All H atoms were placed geometrically and treated as riding on their parent atoms, with thiadiazole C—H and methyl C—H distances at 0.96 Å. The $U_{iso}$(H) values were set at 1.5$U_{eq}$(C) for all H atoms.

**Figures**

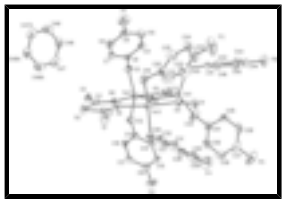

Fig. 1. The structure of the title complex (I), showing 30% probability displacement ellipsoids.

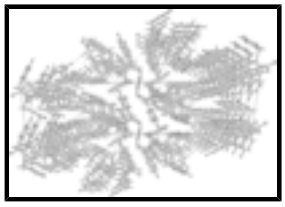

Fig. 2. Unit cell of the title complex (I).

## [$\mu_2$-2,5-Dimercapto-1,3,4-thiadiazole(2-)-$\kappa^2N$:$N$]bis($\mu_2$– methanolato)-$\mu_3$-oxido-tris[bis(4-fluorobenzyl)tin(IV)] benzene hemisolvate

*Crystal data*

| | |
|---|---|
| $[Sn_3(C_7H_7F)_6(CH_3O)_2(C_2N_2S_3)O]\cdot 0.5C_6H_6$ | $F_{000}$ = 2516 |
| $M_r$ = 1276.12 | $D_x$ = 1.702 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Melting point: 356 K |
| Hall symbol: -P 2ybc | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| $a$ = 10.3309 (9) Å | Cell parameters from 9782 reflections |
| $b$ = 45.937 (4) Å | θ = 1.8–26.0º |
| $c$ = 13.5763 (8) Å | μ = 1.68 mm$^{-1}$ |
| β = 129.394 (4)º | $T$ = 293 (2) K |
| $V$ = 4979.1 (7) Å$^3$ | Block, colorless |
| $Z$ = 4 | 0.18 × 0.16 × 0.08 mm |

*Data collection*

| | |
|---|---|
| Siemens SMART CCD area-detector diffractometer | 9782 independent reflections |
| Radiation source: fine-focus sealed tube | 8279 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.048 |
| $T$ = 293(2) K | $\theta_{max}$ = 26.0º |
| φ and ω scans | $\theta_{min}$ = 1.8º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −12→12 |
| $T_{min}$ = 0.751, $T_{max}$ = 0.877 | $k$ = −56→56 |
| 51752 measured reflections | $l$ = −16→16 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.055$ | H-atom parameters constrained |
| $wR(F^2) = 0.184$ | $w = 1/[\sigma^2(F_o^2) + (0.123P)^2 + 12.502P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.02$ | $(\Delta/\sigma)_{max} = 0.003$ |
| 9782 reflections | $\Delta\rho_{max} = 0.72$ e Å$^{-3}$ |
| 591 parameters | $\Delta\rho_{min} = -1.78$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Sn1 | 1.09057 (6) | 0.872437 (11) | 0.26253 (5) | 0.04148 (16) |
| Sn2 | 0.99142 (6) | 0.942464 (10) | 0.27698 (4) | 0.03669 (15) |
| Sn3 | 0.68330 (6) | 0.880017 (10) | 0.12982 (5) | 0.03655 (15) |
| S1 | 0.2941 (3) | 0.90904 (5) | 0.0062 (3) | 0.0677 (6) |
| S2 | 0.4469 (3) | 0.96904 (4) | 0.1112 (2) | 0.0548 (5) |
| S3 | 0.7698 (3) | 1.00416 (5) | 0.2581 (2) | 0.0594 (5) |
| F1 | 0.8398 (10) | 0.88068 (14) | 0.6454 (7) | 0.094 (2) |
| F2 | 0.5363 (10) | 0.91417 (15) | −0.3438 (5) | 0.104 (2) |
| F3 | 0.7676 (14) | 0.74570 (16) | 0.3886 (12) | 0.152 (4) |
| F4 | 0.2991 (11) | 0.76864 (14) | −0.2917 (7) | 0.112 (3) |
| F5 | 0.9696 (12) | 0.77323 (17) | −0.1815 (9) | 0.125 (3) |
| F6 | 1.5752 (11) | 0.75227 (17) | 0.4952 (8) | 0.120 (3) |
| O1 | 0.9093 (5) | 0.90072 (10) | 0.2213 (4) | 0.0384 (10) |
| O2 | 1.1931 (6) | 0.91524 (11) | 0.3167 (5) | 0.0492 (13) |
| O3 | 0.8669 (6) | 0.84801 (11) | 0.1676 (5) | 0.0456 (12) |
| N1 | 0.6135 (7) | 0.92511 (12) | 0.1374 (6) | 0.0386 (13) |
| N2 | 0.7269 (7) | 0.94780 (12) | 0.1975 (5) | 0.0380 (12) |
| C1 | 0.4561 (10) | 0.93234 (17) | 0.0851 (8) | 0.0454 (17) |

| | | | | |
|---|---|---|---|---|
| C2 | 0.6593 (9) | 0.97345 (16) | 0.1925 (7) | 0.0440 (16) |
| C3 | 1.3556 (10) | 0.9245 (2) | 0.3585 (10) | 0.065 (2) |
| H3A | 1.4285 | 0.9080 | 0.3885 | 0.097* |
| H3B | 1.4033 | 0.9385 | 0.4262 | 0.097* |
| H3C | 1.3423 | 0.9333 | 0.2883 | 0.097* |
| C4 | 0.8373 (12) | 0.81699 (16) | 0.1369 (8) | 0.056 (2) |
| H4A | 0.8231 | 0.8135 | 0.0608 | 0.084* |
| H4B | 0.7381 | 0.8111 | 0.1236 | 0.084* |
| H4C | 0.9314 | 0.8060 | 0.2061 | 0.084* |
| C5 | 1.1099 (11) | 0.95023 (19) | 0.4733 (7) | 0.054 (2) |
| H5A | 1.2292 | 0.9467 | 0.5247 | 0.065* |
| H5B | 1.0943 | 0.9705 | 0.4841 | 0.065* |
| C6 | 1.0403 (9) | 0.93103 (17) | 0.5198 (6) | 0.0423 (16) |
| C7 | 0.8973 (11) | 0.93993 (18) | 0.5021 (8) | 0.0502 (18) |
| H7 | 0.8468 | 0.9576 | 0.4622 | 0.060* |
| C8 | 0.8298 (12) | 0.9226 (2) | 0.5436 (9) | 0.063 (2) |
| H8 | 0.7330 | 0.9284 | 0.5294 | 0.076* |
| C9 | 0.9057 (13) | 0.8974 (2) | 0.6044 (8) | 0.062 (2) |
| C10 | 1.0485 (13) | 0.8888 (2) | 0.6276 (8) | 0.064 (2) |
| H10 | 1.1011 | 0.8716 | 0.6716 | 0.077* |
| C11 | 1.1143 (10) | 0.9055 (2) | 0.5860 (7) | 0.056 (2) |
| H11 | 1.2126 | 0.8995 | 0.6029 | 0.067* |
| C12 | 0.9649 (11) | 0.96861 (18) | 0.1346 (7) | 0.0516 (19) |
| H12A | 0.9217 | 0.9876 | 0.1320 | 0.062* |
| H12B | 1.0741 | 0.9714 | 0.1574 | 0.062* |
| C13 | 0.8495 (9) | 0.95493 (15) | 0.0050 (7) | 0.0399 (15) |
| C14 | 0.9149 (11) | 0.9391 (2) | −0.0428 (8) | 0.057 (2) |
| H14 | 1.0302 | 0.9375 | 0.0051 | 0.068* |
| C15 | 0.8075 (14) | 0.9260 (2) | −0.1618 (9) | 0.068 (3) |
| H15 | 0.8498 | 0.9159 | −0.1955 | 0.082* |
| C16 | 0.6388 (13) | 0.9280 (2) | −0.2283 (7) | 0.061 (2) |
| C17 | 0.5720 (11) | 0.94291 (17) | −0.1855 (8) | 0.053 (2) |
| H17 | 0.4564 | 0.9443 | −0.2338 | 0.064* |
| C18 | 0.6791 (10) | 0.95621 (16) | −0.0677 (7) | 0.0450 (17) |
| H18 | 0.6337 | 0.9664 | −0.0368 | 0.054* |
| C19 | 0.6611 (15) | 0.8640 (2) | 0.2674 (11) | 0.070 (3) |
| H19A | 0.7386 | 0.8749 | 0.3458 | 0.084* |
| H19B | 0.5489 | 0.8684 | 0.2364 | 0.084* |
| C20 | 0.6921 (10) | 0.83251 (17) | 0.2988 (7) | 0.0452 (17) |
| C21 | 0.5731 (12) | 0.8119 (2) | 0.2202 (9) | 0.067 (2) |
| H21 | 0.4712 | 0.8178 | 0.1447 | 0.081* |
| C22 | 0.5989 (17) | 0.7829 (2) | 0.2487 (14) | 0.086 (3) |
| H22 | 0.5172 | 0.7693 | 0.1928 | 0.104* |
| C23 | 0.7414 (18) | 0.7745 (2) | 0.3566 (15) | 0.084 (3) |
| C24 | 0.8651 (14) | 0.7927 (3) | 0.4403 (12) | 0.082 (3) |
| H24 | 0.9641 | 0.7858 | 0.5157 | 0.099* |
| C25 | 0.8414 (11) | 0.8229 (2) | 0.4110 (9) | 0.069 (3) |
| H25 | 0.9257 | 0.8361 | 0.4669 | 0.082* |
| C26 | 0.5420 (11) | 0.87894 (17) | −0.0712 (7) | 0.0494 (18) |

| | | | | |
|---|---|---|---|---|
| H26A | 0.4479 | 0.8922 | −0.1101 | 0.059* |
| H26B | 0.6118 | 0.8860 | −0.0907 | 0.059* |
| C27 | 0.4760 (9) | 0.84916 (16) | −0.1307 (7) | 0.0440 (16) |
| C28 | 0.5399 (12) | 0.8352 (2) | −0.1822 (8) | 0.058 (2) |
| H28 | 0.6229 | 0.8440 | −0.1798 | 0.069* |
| C29 | 0.4788 (13) | 0.8078 (2) | −0.2377 (8) | 0.066 (2) |
| H29 | 0.5196 | 0.7984 | −0.2737 | 0.079* |
| C30 | 0.3596 (15) | 0.7950 (2) | −0.2388 (9) | 0.073 (3) |
| C31 | 0.2951 (13) | 0.8087 (2) | −0.1873 (9) | 0.069 (2) |
| H31 | 0.2128 | 0.7997 | −0.1891 | 0.082* |
| C32 | 0.3555 (10) | 0.83586 (18) | −0.1331 (8) | 0.0534 (19) |
| H32 | 0.3136 | 0.8453 | −0.0979 | 0.064* |
| C33 | 1.1616 (14) | 0.8670 (2) | 0.1472 (10) | 0.0653 (18) |
| H33A | 1.1257 | 0.8843 | 0.0947 | 0.078* |
| H33B | 1.2830 | 0.8668 | 0.2038 | 0.078* |
| C34 | 1.1027 (13) | 0.8414 (2) | 0.0609 (10) | 0.0653 (18) |
| C35 | 1.1589 (13) | 0.8136 (2) | 0.1060 (9) | 0.066 (2) |
| H35 | 1.2299 | 0.8102 | 0.1934 | 0.079* |
| C36 | 1.1128 (14) | 0.7909 (2) | 0.0253 (11) | 0.074 (3) |
| H36 | 1.1493 | 0.7721 | 0.0569 | 0.089* |
| C37 | 1.0143 (14) | 0.7959 (2) | −0.0998 (11) | 0.073 (3) |
| C38 | 0.9535 (16) | 0.8222 (3) | −0.1497 (11) | 0.089 (3) |
| H38 | 0.8808 | 0.8249 | −0.2375 | 0.107* |
| C39 | 1.0005 (14) | 0.8453 (2) | −0.0687 (10) | 0.072 (3) |
| H39 | 0.9623 | 0.8639 | −0.1024 | 0.087* |
| C40 | 1.2385 (11) | 0.8535 (2) | 0.4489 (8) | 0.060 (2) |
| H40A | 1.3207 | 0.8676 | 0.5105 | 0.072* |
| H40B | 1.1664 | 0.8490 | 0.4695 | 0.072* |
| C41 | 1.3267 (10) | 0.82649 (17) | 0.4604 (7) | 0.0479 (17) |
| C42 | 1.4822 (11) | 0.8276 (2) | 0.4905 (9) | 0.062 (2) |
| H42 | 1.5316 | 0.8456 | 0.5031 | 0.075* |
| C43 | 1.5658 (13) | 0.8028 (3) | 0.5021 (10) | 0.077 (3) |
| H43 | 1.6709 | 0.8040 | 0.5236 | 0.092* |
| C44 | 1.4915 (17) | 0.7767 (3) | 0.4816 (10) | 0.080 (3) |
| C45 | 1.3412 (15) | 0.7739 (2) | 0.4501 (10) | 0.079 (3) |
| H45 | 1.2937 | 0.7556 | 0.4359 | 0.095* |
| C46 | 1.2565 (12) | 0.7988 (2) | 0.4388 (8) | 0.062 (2) |
| H46 | 1.1511 | 0.7971 | 0.4164 | 0.074* |
| C47 | 0.5586 (14) | 1.0005 (2) | 0.4335 (10) | 0.069 (3) |
| H47 | 0.5976 | 1.0009 | 0.3878 | 0.082* |
| C48 | 0.6669 (13) | 0.99371 (17) | 0.5618 (10) | 0.060 (2) |
| H48 | 0.7787 | 0.9895 | 0.6031 | 0.072* |
| C49 | 0.6062 (14) | 0.9934 (2) | 0.6267 (9) | 0.070 (3) |
| H49 | 0.6780 | 0.9889 | 0.7131 | 0.084* |

*Atomic displacement parameters (Å$^2$)*

| $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| Sn1 | 0.0409 (3) | 0.0400 (3) | 0.0480 (3) | 0.0006 (2) | 0.0303 (2) | −0.0030 (2) |
| Sn2 | 0.0393 (3) | 0.0357 (3) | 0.0343 (3) | −0.00752 (19) | 0.0230 (2) | −0.00782 (18) |
| Sn3 | 0.0391 (3) | 0.0312 (3) | 0.0435 (3) | −0.00509 (18) | 0.0282 (2) | −0.00437 (18) |
| S1 | 0.0481 (11) | 0.0596 (13) | 0.1021 (19) | −0.0090 (10) | 0.0509 (13) | −0.0123 (12) |
| S2 | 0.0542 (11) | 0.0422 (10) | 0.0713 (14) | 0.0074 (9) | 0.0413 (11) | −0.0030 (9) |
| S3 | 0.0691 (14) | 0.0409 (10) | 0.0666 (13) | −0.0066 (9) | 0.0423 (12) | −0.0162 (9) |
| F1 | 0.134 (6) | 0.089 (4) | 0.103 (5) | −0.019 (4) | 0.096 (5) | 0.004 (4) |
| F2 | 0.127 (6) | 0.101 (5) | 0.041 (3) | −0.002 (4) | 0.033 (3) | −0.019 (3) |
| F3 | 0.208 (10) | 0.067 (5) | 0.267 (12) | 0.047 (5) | 0.190 (10) | 0.052 (6) |
| F4 | 0.156 (7) | 0.060 (4) | 0.091 (5) | −0.026 (4) | 0.065 (5) | −0.032 (3) |
| F5 | 0.171 (8) | 0.099 (5) | 0.151 (7) | −0.044 (5) | 0.123 (7) | −0.065 (5) |
| F6 | 0.142 (7) | 0.101 (5) | 0.115 (6) | 0.059 (5) | 0.080 (5) | 0.009 (4) |
| O1 | 0.033 (2) | 0.032 (2) | 0.045 (3) | −0.0005 (18) | 0.022 (2) | −0.0051 (19) |
| O2 | 0.037 (3) | 0.050 (3) | 0.062 (3) | −0.009 (2) | 0.032 (3) | −0.015 (3) |
| O3 | 0.046 (3) | 0.035 (3) | 0.062 (3) | −0.003 (2) | 0.037 (3) | −0.005 (2) |
| N1 | 0.041 (3) | 0.034 (3) | 0.052 (3) | −0.001 (2) | 0.035 (3) | −0.004 (2) |
| N2 | 0.037 (3) | 0.035 (3) | 0.039 (3) | −0.002 (2) | 0.023 (3) | −0.007 (2) |
| C1 | 0.047 (4) | 0.044 (4) | 0.059 (5) | 0.001 (3) | 0.040 (4) | 0.003 (3) |
| C2 | 0.048 (4) | 0.042 (4) | 0.045 (4) | 0.003 (3) | 0.031 (4) | −0.006 (3) |
| C3 | 0.044 (4) | 0.066 (6) | 0.092 (7) | −0.005 (4) | 0.047 (5) | −0.005 (5) |
| C4 | 0.069 (5) | 0.036 (4) | 0.062 (5) | 0.016 (4) | 0.041 (5) | −0.001 (4) |
| C5 | 0.057 (5) | 0.061 (5) | 0.040 (4) | −0.013 (4) | 0.028 (4) | −0.017 (4) |
| C6 | 0.042 (4) | 0.052 (4) | 0.028 (3) | −0.002 (3) | 0.020 (3) | −0.008 (3) |
| C7 | 0.057 (5) | 0.052 (5) | 0.048 (4) | 0.003 (4) | 0.037 (4) | 0.002 (3) |
| C8 | 0.065 (5) | 0.081 (6) | 0.064 (5) | 0.000 (5) | 0.050 (5) | −0.002 (5) |
| C9 | 0.086 (7) | 0.058 (5) | 0.053 (5) | −0.013 (5) | 0.049 (5) | −0.001 (4) |
| C10 | 0.079 (6) | 0.054 (5) | 0.050 (5) | 0.006 (5) | 0.037 (5) | 0.005 (4) |
| C11 | 0.046 (4) | 0.072 (6) | 0.035 (4) | 0.004 (4) | 0.019 (4) | 0.000 (4) |
| C12 | 0.058 (5) | 0.050 (4) | 0.050 (4) | −0.005 (4) | 0.036 (4) | 0.003 (4) |
| C13 | 0.049 (4) | 0.036 (3) | 0.040 (4) | 0.006 (3) | 0.031 (3) | 0.005 (3) |
| C14 | 0.054 (5) | 0.074 (6) | 0.044 (4) | 0.020 (4) | 0.032 (4) | 0.008 (4) |
| C15 | 0.099 (8) | 0.070 (6) | 0.052 (5) | 0.028 (5) | 0.056 (6) | 0.007 (4) |
| C16 | 0.076 (6) | 0.055 (5) | 0.032 (4) | 0.006 (4) | 0.025 (4) | 0.003 (3) |
| C17 | 0.046 (4) | 0.049 (5) | 0.045 (4) | 0.005 (3) | 0.019 (4) | 0.014 (3) |
| C18 | 0.053 (4) | 0.043 (4) | 0.050 (4) | 0.009 (3) | 0.038 (4) | 0.007 (3) |
| C19 | 0.103 (8) | 0.062 (6) | 0.088 (7) | 0.010 (5) | 0.080 (7) | 0.012 (5) |
| C20 | 0.054 (4) | 0.046 (4) | 0.053 (4) | −0.007 (3) | 0.042 (4) | −0.002 (3) |
| C21 | 0.055 (5) | 0.073 (6) | 0.058 (5) | −0.017 (5) | 0.029 (4) | 0.002 (5) |
| C22 | 0.101 (9) | 0.062 (7) | 0.124 (10) | −0.026 (6) | 0.085 (9) | −0.014 (7) |
| C23 | 0.105 (9) | 0.051 (6) | 0.141 (11) | 0.010 (6) | 0.099 (9) | 0.022 (7) |
| C24 | 0.069 (6) | 0.092 (8) | 0.105 (8) | 0.033 (6) | 0.064 (7) | 0.049 (7) |
| C25 | 0.050 (5) | 0.085 (7) | 0.065 (6) | −0.019 (5) | 0.034 (5) | −0.005 (5) |
| C26 | 0.057 (5) | 0.045 (4) | 0.044 (4) | −0.007 (3) | 0.032 (4) | −0.001 (3) |
| C27 | 0.043 (4) | 0.043 (4) | 0.038 (4) | −0.003 (3) | 0.022 (3) | −0.002 (3) |
| C28 | 0.064 (5) | 0.066 (5) | 0.050 (5) | 0.002 (4) | 0.039 (4) | −0.005 (4) |
| C29 | 0.086 (7) | 0.062 (6) | 0.047 (5) | 0.007 (5) | 0.040 (5) | −0.007 (4) |
| C30 | 0.099 (8) | 0.046 (5) | 0.054 (5) | −0.004 (5) | 0.039 (6) | −0.013 (4) |
| C31 | 0.068 (6) | 0.057 (5) | 0.065 (6) | −0.016 (5) | 0.035 (5) | −0.009 (4) |
| C32 | 0.052 (4) | 0.050 (4) | 0.050 (4) | −0.008 (4) | 0.028 (4) | −0.006 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C33 | 0.087 (5) | 0.062 (4) | 0.088 (5) | −0.019 (3) | 0.075 (4) | −0.016 (3) |
| C34 | 0.087 (5) | 0.062 (4) | 0.088 (5) | −0.019 (3) | 0.075 (4) | −0.016 (3) |
| C35 | 0.078 (6) | 0.073 (6) | 0.056 (5) | 0.014 (5) | 0.047 (5) | 0.011 (4) |
| C36 | 0.098 (8) | 0.050 (5) | 0.104 (8) | 0.020 (5) | 0.078 (7) | 0.017 (5) |
| C37 | 0.081 (7) | 0.071 (6) | 0.092 (8) | −0.018 (5) | 0.066 (7) | −0.027 (6) |
| C38 | 0.094 (8) | 0.101 (9) | 0.054 (6) | 0.001 (7) | 0.038 (6) | −0.001 (6) |
| C39 | 0.089 (7) | 0.061 (6) | 0.070 (6) | 0.022 (5) | 0.052 (6) | 0.022 (5) |
| C40 | 0.060 (5) | 0.071 (6) | 0.048 (5) | 0.008 (4) | 0.034 (4) | −0.002 (4) |
| C41 | 0.051 (4) | 0.052 (5) | 0.038 (4) | 0.005 (3) | 0.027 (4) | 0.006 (3) |
| C42 | 0.049 (5) | 0.074 (6) | 0.059 (5) | −0.007 (4) | 0.032 (4) | −0.005 (4) |
| C43 | 0.053 (5) | 0.101 (9) | 0.072 (6) | 0.019 (5) | 0.038 (5) | −0.004 (6) |
| C44 | 0.101 (9) | 0.072 (7) | 0.056 (6) | 0.033 (6) | 0.045 (6) | 0.003 (5) |
| C45 | 0.090 (8) | 0.051 (5) | 0.067 (6) | −0.003 (5) | 0.036 (6) | 0.000 (5) |
| C46 | 0.063 (5) | 0.078 (6) | 0.043 (4) | 0.006 (5) | 0.032 (4) | 0.008 (4) |
| C47 | 0.090 (7) | 0.057 (5) | 0.087 (7) | −0.032 (5) | 0.069 (6) | −0.022 (5) |
| C48 | 0.070 (6) | 0.039 (4) | 0.083 (7) | −0.005 (4) | 0.054 (5) | −0.003 (4) |
| C49 | 0.080 (7) | 0.061 (6) | 0.057 (5) | −0.015 (5) | 0.037 (5) | 0.000 (4) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Sn1—O1 | 2.044 (4) | C18—H18 | 0.9300 |
| Sn1—O3 | 2.116 (5) | C19—C20 | 1.486 (12) |
| Sn1—C33 | 2.125 (8) | C19—H19A | 0.9700 |
| Sn1—O2 | 2.131 (5) | C19—H19B | 0.9700 |
| Sn1—C40 | 2.142 (9) | C20—C21 | 1.373 (12) |
| Sn2—O1 | 2.038 (5) | C20—C25 | 1.383 (12) |
| Sn2—C12 | 2.141 (7) | C21—C22 | 1.366 (15) |
| Sn2—C5 | 2.142 (7) | C21—H21 | 0.9300 |
| Sn2—O2 | 2.184 (5) | C22—C23 | 1.312 (17) |
| Sn2—N2 | 2.225 (6) | C22—H22 | 0.9300 |
| Sn3—O1 | 2.054 (4) | C23—C24 | 1.334 (18) |
| Sn3—C26 | 2.127 (8) | C24—C25 | 1.419 (15) |
| Sn3—C19 | 2.150 (8) | C24—H24 | 0.9300 |
| Sn3—O3 | 2.188 (5) | C25—H25 | 0.9300 |
| Sn3—N1 | 2.217 (5) | C26—C27 | 1.513 (10) |
| S1—C1 | 1.679 (8) | C26—H26A | 0.9700 |
| S2—C2 | 1.732 (8) | C26—H26B | 0.9700 |
| S2—C1 | 1.738 (8) | C27—C32 | 1.369 (11) |
| S3—C2 | 1.672 (8) | C27—C28 | 1.386 (11) |
| F1—C9 | 1.358 (10) | C28—C29 | 1.394 (13) |
| F2—C16 | 1.370 (10) | C28—H28 | 0.9300 |
| F3—C23 | 1.367 (12) | C29—C30 | 1.357 (15) |
| F4—C30 | 1.342 (11) | C29—H29 | 0.9300 |
| F5—C37 | 1.371 (11) | C30—C31 | 1.386 (15) |
| F6—C44 | 1.357 (11) | C31—C32 | 1.381 (12) |
| O2—C3 | 1.454 (9) | C31—H31 | 0.9300 |
| O3—C4 | 1.462 (9) | C32—H32 | 0.9300 |
| N1—C1 | 1.339 (9) | C33—C34 | 1.488 (12) |
| N1—N2 | 1.382 (8) | C33—H33A | 0.9700 |

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|---|---|---|---|
| N2—C2 | 1.349 (9) | C33—H33B | 0.9700 |
| C3—H3A | 0.9600 | C34—C39 | 1.373 (14) |
| C3—H3B | 0.9600 | C34—C35 | 1.377 (13) |
| C3—H3C | 0.9600 | C35—C36 | 1.360 (14) |
| C4—H4A | 0.9600 | C35—H35 | 0.9300 |
| C4—H4B | 0.9600 | C36—C37 | 1.334 (15) |
| C4—H4C | 0.9600 | C36—H36 | 0.9300 |
| C5—C6 | 1.506 (11) | C37—C38 | 1.331 (16) |
| C5—H5A | 0.9700 | C38—C39 | 1.375 (15) |
| C5—H5B | 0.9700 | C38—H38 | 0.9300 |
| C6—C11 | 1.376 (12) | C39—H39 | 0.9300 |
| C6—C7 | 1.399 (11) | C40—C41 | 1.487 (12) |
| C7—C8 | 1.390 (12) | C40—H40A | 0.9700 |
| C7—H7 | 0.9300 | C40—H40B | 0.9700 |
| C8—C9 | 1.348 (13) | C41—C42 | 1.385 (12) |
| C8—H8 | 0.9300 | C41—C46 | 1.399 (12) |
| C9—C10 | 1.357 (14) | C42—C43 | 1.375 (14) |
| C10—C11 | 1.363 (13) | C42—H42 | 0.9300 |
| C10—H10 | 0.9300 | C43—C44 | 1.353 (17) |
| C11—H11 | 0.9300 | C43—H43 | 0.9300 |
| C12—C13 | 1.500 (11) | C44—C45 | 1.330 (16) |
| C12—H12A | 0.9700 | C45—C46 | 1.389 (14) |
| C12—H12B | 0.9700 | C45—H45 | 0.9300 |
| C13—C18 | 1.368 (10) | C46—H46 | 0.9300 |
| C13—C14 | 1.400 (10) | C47—C49$^{i}$ | 1.372 (15) |
| C14—C15 | 1.391 (13) | C47—C48 | 1.381 (14) |
| C14—H14 | 0.9300 | C47—H47 | 0.9300 |
| C15—C16 | 1.366 (14) | C48—C49 | 1.368 (13) |
| C15—H15 | 0.9300 | C48—H48 | 0.9300 |
| C16—C17 | 1.338 (13) | C49—C47$^{i}$ | 1.372 (15) |
| C17—C18 | 1.382 (11) | C49—H49 | 0.9300 |
| C17—H17 | 0.9300 | | |
| O1—Sn1—O3 | 73.36 (18) | C13—C18—C17 | 122.3 (7) |
| O1—Sn1—C33 | 123.9 (3) | C13—C18—H18 | 118.8 |
| O3—Sn1—C33 | 104.1 (3) | C17—C18—H18 | 118.8 |
| O1—Sn1—O2 | 71.11 (18) | C20—C19—Sn3 | 117.4 (6) |
| O3—Sn1—O2 | 144.2 (2) | C20—C19—H19A | 108.0 |
| C33—Sn1—O2 | 92.0 (3) | Sn3—C19—H19A | 108.0 |
| O1—Sn1—C40 | 115.1 (3) | C20—C19—H19B | 108.0 |
| O3—Sn1—C40 | 100.9 (3) | Sn3—C19—H19B | 108.0 |
| C33—Sn1—C40 | 120.1 (4) | H19A—C19—H19B | 107.2 |
| O2—Sn1—C40 | 98.1 (3) | C21—C20—C25 | 117.3 (8) |
| O1—Sn2—C12 | 114.1 (3) | C21—C20—C19 | 121.8 (9) |
| O1—Sn2—C5 | 113.1 (3) | C25—C20—C19 | 121.0 (8) |
| C12—Sn2—C5 | 132.4 (3) | C22—C21—C20 | 122.4 (10) |
| O1—Sn2—O2 | 70.13 (18) | C22—C21—H21 | 118.8 |
| C12—Sn2—O2 | 95.7 (3) | C20—C21—H21 | 118.8 |
| C5—Sn2—O2 | 94.9 (3) | C23—C22—C21 | 118.6 (11) |

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| O1—Sn2—N2 | 80.20 (19) | C23—C22—H22 | 120.7 |
| C12—Sn2—N2 | 95.0 (3) | C21—C22—H22 | 120.7 |
| C5—Sn2—N2 | 98.1 (3) | C22—C23—C24 | 124.0 (10) |
| O2—Sn2—N2 | 150.29 (19) | C22—C23—F3 | 119.5 (13) |
| O1—Sn3—C26 | 112.2 (3) | C24—C23—F3 | 116.5 (13) |
| O1—Sn3—C19 | 109.9 (4) | C23—C24—C25 | 118.1 (10) |
| C26—Sn3—C19 | 137.9 (4) | C23—C24—H24 | 121.0 |
| O1—Sn3—O3 | 71.67 (18) | C25—C24—H24 | 121.0 |
| C26—Sn3—O3 | 94.1 (3) | C20—C25—C24 | 119.6 (9) |
| C19—Sn3—O3 | 97.0 (3) | C20—C25—H25 | 120.2 |
| O1—Sn3—N1 | 79.50 (19) | C24—C25—H25 | 120.2 |
| C26—Sn3—N1 | 95.9 (3) | C27—C26—Sn3 | 114.6 (5) |
| C19—Sn3—N1 | 93.6 (3) | C27—C26—H26A | 108.6 |
| O3—Sn3—N1 | 151.2 (2) | Sn3—C26—H26A | 108.6 |
| C2—S2—C1 | 91.9 (4) | C27—C26—H26B | 108.6 |
| Sn2—O1—Sn1 | 113.8 (2) | Sn3—C26—H26B | 108.6 |
| Sn2—O1—Sn3 | 134.9 (2) | H26A—C26—H26B | 107.6 |
| Sn1—O1—Sn3 | 111.3 (2) | C32—C27—C28 | 119.9 (8) |
| C3—O2—Sn1 | 127.1 (5) | C32—C27—C26 | 120.7 (7) |
| C3—O2—Sn2 | 127.8 (5) | C28—C27—C26 | 119.4 (7) |
| Sn1—O2—Sn2 | 104.8 (2) | C27—C28—C29 | 119.6 (9) |
| C4—O3—Sn1 | 129.8 (5) | C27—C28—H28 | 120.2 |
| C4—O3—Sn3 | 126.5 (5) | C29—C28—H28 | 120.2 |
| Sn1—O3—Sn3 | 103.6 (2) | C30—C29—C28 | 119.6 (9) |
| C1—N1—N2 | 114.5 (6) | C30—C29—H29 | 120.2 |
| C1—N1—Sn3 | 121.9 (5) | C28—C29—H29 | 120.2 |
| N2—N1—Sn3 | 123.6 (4) | F4—C30—C29 | 120.6 (10) |
| C2—N2—N1 | 114.3 (6) | F4—C30—C31 | 118.0 (11) |
| C2—N2—Sn2 | 123.9 (5) | C29—C30—C31 | 121.4 (9) |
| N1—N2—Sn2 | 121.5 (4) | C32—C31—C30 | 118.7 (9) |
| N1—C1—S1 | 124.3 (6) | C32—C31—H31 | 120.7 |
| N1—C1—S2 | 109.7 (5) | C30—C31—H31 | 120.7 |
| S1—C1—S2 | 126.0 (5) | C27—C32—C31 | 120.9 (9) |
| N2—C2—S3 | 123.6 (6) | C27—C32—H32 | 119.6 |
| N2—C2—S2 | 109.6 (5) | C31—C32—H32 | 119.6 |
| S3—C2—S2 | 126.8 (4) | C34—C33—Sn1 | 120.9 (6) |
| O2—C3—H3A | 109.5 | C34—C33—H33A | 107.1 |
| O2—C3—H3B | 109.5 | Sn1—C33—H33A | 107.1 |
| H3A—C3—H3B | 109.5 | C34—C33—H33B | 107.1 |
| O2—C3—H3C | 109.5 | Sn1—C33—H33B | 107.1 |
| H3A—C3—H3C | 109.5 | H33A—C33—H33B | 106.8 |
| H3B—C3—H3C | 109.5 | C39—C34—C35 | 117.0 (9) |
| O3—C4—H4A | 109.5 | C39—C34—C33 | 120.3 (9) |
| O3—C4—H4B | 109.5 | C35—C34—C33 | 122.5 (10) |
| H4A—C4—H4B | 109.5 | C36—C35—C34 | 121.4 (9) |
| O3—C4—H4C | 109.5 | C36—C35—H35 | 119.3 |
| H4A—C4—H4C | 109.5 | C34—C35—H35 | 119.3 |
| H4B—C4—H4C | 109.5 | C37—C36—C35 | 119.1 (9) |
| C6—C5—Sn2 | 112.1 (5) | C37—C36—H36 | 120.4 |

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| C6—C5—H5A | 109.2 | C35—C36—H36 | 120.4 |
| Sn2—C5—H5A | 109.2 | C38—C37—C36 | 122.5 (10) |
| C6—C5—H5B | 109.2 | C38—C37—F5 | 118.1 (11) |
| Sn2—C5—H5B | 109.2 | C36—C37—F5 | 119.4 (11) |
| H5A—C5—H5B | 107.9 | C37—C38—C39 | 118.6 (10) |
| C11—C6—C7 | 116.7 (7) | C37—C38—H38 | 120.7 |
| C11—C6—C5 | 123.9 (7) | C39—C38—H38 | 120.7 |
| C7—C6—C5 | 119.3 (7) | C34—C39—C38 | 121.3 (10) |
| C8—C7—C6 | 120.6 (8) | C34—C39—H39 | 119.3 |
| C8—C7—H7 | 119.7 | C38—C39—H39 | 119.3 |
| C6—C7—H7 | 119.7 | C41—C40—Sn1 | 113.2 (5) |
| C9—C8—C7 | 119.6 (9) | C41—C40—H40A | 108.9 |
| C9—C8—H8 | 120.2 | Sn1—C40—H40A | 108.9 |
| C7—C8—H8 | 120.2 | C41—C40—H40B | 108.9 |
| C8—C9—C10 | 121.1 (8) | Sn1—C40—H40B | 108.9 |
| C8—C9—F1 | 119.3 (9) | H40A—C40—H40B | 107.8 |
| C10—C9—F1 | 119.6 (9) | C42—C41—C46 | 116.4 (8) |
| C9—C10—C11 | 119.6 (9) | C42—C41—C40 | 121.3 (8) |
| C9—C10—H10 | 120.2 | C46—C41—C40 | 122.3 (8) |
| C11—C10—H10 | 120.2 | C43—C42—C41 | 122.0 (9) |
| C10—C11—C6 | 122.3 (8) | C43—C42—H42 | 119.0 |
| C10—C11—H11 | 118.9 | C41—C42—H42 | 119.0 |
| C6—C11—H11 | 118.9 | C44—C43—C42 | 118.4 (10) |
| C13—C12—Sn2 | 112.0 (5) | C44—C43—H43 | 120.8 |
| C13—C12—H12A | 109.2 | C42—C43—H43 | 120.8 |
| Sn2—C12—H12A | 109.2 | C45—C44—C43 | 123.2 (10) |
| C13—C12—H12B | 109.2 | C45—C44—F6 | 118.4 (12) |
| Sn2—C12—H12B | 109.2 | C43—C44—F6 | 118.5 (12) |
| H12A—C12—H12B | 107.9 | C44—C45—C46 | 118.7 (10) |
| C18—C13—C14 | 117.8 (7) | C44—C45—H45 | 120.7 |
| C18—C13—C12 | 122.0 (7) | C46—C45—H45 | 120.7 |
| C14—C13—C12 | 120.1 (7) | C45—C46—C41 | 121.3 (9) |
| C15—C14—C13 | 120.0 (8) | C45—C46—H46 | 119.3 |
| C15—C14—H14 | 120.0 | C41—C46—H46 | 119.3 |
| C13—C14—H14 | 120.0 | C49$^{i}$—C47—C48 | 120.2 (9) |
| C16—C15—C14 | 118.7 (8) | C49$^{i}$—C47—H47 | 119.9 |
| C16—C15—H15 | 120.7 | C48—C47—H47 | 119.9 |
| C14—C15—H15 | 120.7 | C49—C48—C47 | 118.7 (9) |
| C17—C16—C15 | 122.8 (8) | C49—C48—H48 | 120.7 |
| C17—C16—F2 | 119.8 (9) | C47—C48—H48 | 120.7 |
| C15—C16—F2 | 117.4 (9) | C48—C49—C47$^{i}$ | 121.1 (9) |
| C16—C17—C18 | 118.3 (8) | C48—C49—H49 | 119.4 |
| C16—C17—H17 | 120.9 | C47$^{i}$—C49—H49 | 119.4 |
| C18—C17—H17 | 120.9 | | |
| C12—Sn2—O1—Sn1 | 90.6 (3) | Sn2—C5—C6—C7 | −86.0 (8) |
| C5—Sn2—O1—Sn1 | −83.6 (3) | C11—C6—C7—C8 | −3.7 (12) |
| O2—Sn2—O1—Sn1 | 3.2 (2) | C5—C6—C7—C8 | 179.8 (7) |
| N2—Sn2—O1—Sn1 | −178.3 (3) | C6—C7—C8—C9 | 1.8 (13) |

| | | | |
|---|---|---|---|
| C12—Sn2—O1—Sn3 | −88.3 (4) | C7—C8—C9—C10 | 1.0 (14) |
| C5—Sn2—O1—Sn3 | 97.5 (4) | C7—C8—C9—F1 | 179.6 (8) |
| O2—Sn2—O1—Sn3 | −175.7 (4) | C8—C9—C10—C11 | −1.7 (14) |
| N2—Sn2—O1—Sn3 | 2.8 (3) | F1—C9—C10—C11 | 179.7 (8) |
| O3—Sn1—O1—Sn2 | −178.6 (3) | C9—C10—C11—C6 | −0.4 (13) |
| C33—Sn1—O1—Sn2 | −82.6 (4) | C7—C6—C11—C10 | 3.0 (12) |
| O2—Sn1—O1—Sn2 | −3.3 (2) | C5—C6—C11—C10 | 179.4 (7) |
| C40—Sn1—O1—Sn2 | 87.0 (4) | O1—Sn2—C12—C13 | 15.3 (7) |
| O3—Sn1—O1—Sn3 | 0.6 (2) | C5—Sn2—C12—C13 | −171.9 (5) |
| C33—Sn1—O1—Sn3 | 96.6 (4) | O2—Sn2—C12—C13 | 86.1 (6) |
| O2—Sn1—O1—Sn3 | 175.9 (3) | N2—Sn2—C12—C13 | −66.2 (6) |
| C40—Sn1—O1—Sn3 | −93.8 (4) | Sn2—C12—C13—C18 | 78.7 (8) |
| C26—Sn3—O1—Sn2 | 91.4 (4) | Sn2—C12—C13—C14 | −98.4 (8) |
| C19—Sn3—O1—Sn2 | −90.7 (4) | C18—C13—C14—C15 | 1.5 (12) |
| O3—Sn3—O1—Sn2 | 178.4 (4) | C12—C13—C14—C15 | 178.6 (8) |
| N1—Sn3—O1—Sn2 | −0.7 (3) | C13—C14—C15—C16 | −2.0 (14) |
| C26—Sn3—O1—Sn1 | −87.5 (3) | C14—C15—C16—C17 | 2.0 (15) |
| C19—Sn3—O1—Sn1 | 90.4 (3) | C14—C15—C16—F2 | −178.3 (8) |
| O3—Sn3—O1—Sn1 | −0.6 (2) | C15—C16—C17—C18 | −1.3 (13) |
| N1—Sn3—O1—Sn1 | −179.6 (3) | F2—C16—C17—C18 | 178.9 (8) |
| O1—Sn1—O2—C3 | −171.4 (7) | C14—C13—C18—C17 | −0.9 (11) |
| O3—Sn1—O2—C3 | −163.7 (6) | C12—C13—C18—C17 | −178.0 (7) |
| C33—Sn1—O2—C3 | −46.1 (7) | C16—C17—C18—C13 | 0.8 (12) |
| C40—Sn1—O2—C3 | 74.7 (7) | O1—Sn3—C19—C20 | −101.4 (8) |
| O1—Sn1—O2—Sn2 | 2.9 (2) | C26—Sn3—C19—C20 | 75.6 (10) |
| O3—Sn1—O2—Sn2 | 10.6 (5) | O3—Sn3—C19—C20 | −28.5 (8) |
| C33—Sn1—O2—Sn2 | 128.3 (4) | N1—Sn3—C19—C20 | 178.4 (8) |
| C40—Sn1—O2—Sn2 | −111.0 (3) | Sn3—C19—C20—C21 | −78.9 (10) |
| O1—Sn2—O2—C3 | 171.3 (7) | Sn3—C19—C20—C25 | 102.9 (9) |
| C12—Sn2—O2—C3 | 57.8 (7) | C25—C20—C21—C22 | −0.8 (14) |
| C5—Sn2—O2—C3 | −75.8 (7) | C19—C20—C21—C22 | −179.0 (9) |
| N2—Sn2—O2—C3 | 168.3 (6) | C20—C21—C22—C23 | 1.5 (17) |
| O1—Sn2—O2—Sn1 | −2.9 (2) | C21—C22—C23—C24 | −1.0 (19) |
| C12—Sn2—O2—Sn1 | −116.5 (3) | C21—C22—C23—F3 | 178.0 (10) |
| C5—Sn2—O2—Sn1 | 109.9 (3) | C22—C23—C24—C25 | −0.1 (18) |
| N2—Sn2—O2—Sn1 | −6.0 (5) | F3—C23—C24—C25 | −179.1 (9) |
| O1—Sn1—O3—C4 | −178.4 (7) | C21—C20—C25—C24 | −0.3 (13) |
| C33—Sn1—O3—C4 | 59.9 (7) | C19—C20—C25—C24 | 177.9 (8) |
| O2—Sn1—O3—C4 | 174.0 (6) | C23—C24—C25—C20 | 0.8 (15) |
| C40—Sn1—O3—C4 | −65.2 (7) | O1—Sn3—C26—C27 | 129.7 (5) |
| O1—Sn1—O3—Sn3 | −0.52 (19) | C19—Sn3—C26—C27 | −47.3 (8) |
| C33—Sn1—O3—Sn3 | −122.2 (3) | O3—Sn3—C26—C27 | 57.9 (6) |
| O2—Sn1—O3—Sn3 | −8.1 (5) | N1—Sn3—C26—C27 | −149.2 (6) |
| C40—Sn1—O3—Sn3 | 112.7 (3) | Sn3—C26—C27—C32 | 67.6 (9) |
| O1—Sn3—O3—C4 | 178.5 (6) | Sn3—C26—C27—C28 | −111.9 (7) |
| C26—Sn3—O3—C4 | −69.5 (6) | C32—C27—C28—C29 | 0.9 (12) |
| C19—Sn3—O3—C4 | 69.8 (7) | C26—C27—C28—C29 | −179.7 (8) |
| N1—Sn3—O3—C4 | −179.7 (5) | C27—C28—C29—C30 | −1.0 (14) |
| O1—Sn3—O3—Sn1 | 0.5 (2) | C28—C29—C30—F4 | 180.0 (9) |

| | | | |
|---|---|---|---|
| C26—Sn3—O3—Sn1 | 112.6 (3) | C28—C29—C30—C31 | 0.9 (15) |
| C19—Sn3—O3—Sn1 | −108.2 (4) | F4—C30—C31—C32 | −179.6 (9) |
| N1—Sn3—O3—Sn1 | 2.4 (6) | C29—C30—C31—C32 | −0.5 (15) |
| O1—Sn3—N1—C1 | 177.6 (6) | C28—C27—C32—C31 | −0.5 (13) |
| C26—Sn3—N1—C1 | 66.1 (6) | C26—C27—C32—C31 | −179.9 (8) |
| C19—Sn3—N1—C1 | −72.8 (6) | C30—C31—C32—C27 | 0.3 (14) |
| O3—Sn3—N1—C1 | 175.8 (5) | O1—Sn1—C33—C34 | −102.5 (9) |
| O1—Sn3—N1—N2 | −3.7 (5) | O3—Sn1—C33—C34 | −23.2 (10) |
| C26—Sn3—N1—N2 | −115.2 (5) | O2—Sn1—C33—C34 | −170.9 (9) |
| C19—Sn3—N1—N2 | 105.9 (6) | C40—Sn1—C33—C34 | 88.5 (10) |
| O3—Sn3—N1—N2 | −5.5 (8) | Sn1—C33—C34—C39 | 116.1 (9) |
| C1—N1—N2—C2 | −0.4 (9) | Sn1—C33—C34—C35 | −70.0 (12) |
| Sn3—N1—N2—C2 | −179.2 (5) | C39—C34—C35—C36 | −1.1 (15) |
| C1—N1—N2—Sn2 | −174.6 (5) | C33—C34—C35—C36 | −175.1 (9) |
| Sn3—N1—N2—Sn2 | 6.6 (7) | C34—C35—C36—C37 | 1.7 (16) |
| O1—Sn2—N2—C2 | −178.7 (6) | C35—C36—C37—C38 | −2.8 (17) |
| C12—Sn2—N2—C2 | −65.0 (6) | C35—C36—C37—F5 | 178.9 (9) |
| C5—Sn2—N2—C2 | 69.1 (6) | C36—C37—C38—C39 | 3.2 (19) |
| O2—Sn2—N2—C2 | −175.8 (5) | F5—C37—C38—C39 | −178.5 (10) |
| O1—Sn2—N2—N1 | −5.1 (5) | C35—C34—C39—C38 | 1.5 (16) |
| C12—Sn2—N2—N1 | 108.5 (5) | C33—C34—C39—C38 | 175.7 (10) |
| C5—Sn2—N2—N1 | −117.3 (5) | C37—C38—C39—C34 | −2.5 (19) |
| O2—Sn2—N2—N1 | −2.2 (8) | O1—Sn1—C40—C41 | 160.7 (6) |
| N2—N1—C1—S1 | 179.8 (5) | O3—Sn1—C40—C41 | 84.1 (7) |
| Sn3—N1—C1—S1 | −1.4 (9) | C33—Sn1—C40—C41 | −29.3 (8) |
| N2—N1—C1—S2 | 0.0 (8) | O2—Sn1—C40—C41 | −126.4 (6) |
| Sn3—N1—C1—S2 | 178.8 (3) | Sn1—C40—C41—C42 | 86.6 (9) |
| C2—S2—C1—N1 | 0.3 (6) | Sn1—C40—C41—C46 | −91.9 (8) |
| C2—S2—C1—S1 | −179.5 (6) | C46—C41—C42—C43 | −1.8 (13) |
| N1—N2—C2—S3 | 179.9 (5) | C40—C41—C42—C43 | 179.7 (8) |
| Sn2—N2—C2—S3 | −6.1 (9) | C41—C42—C43—C44 | 1.0 (15) |
| N1—N2—C2—S2 | 0.6 (8) | C42—C43—C44—C45 | 0.3 (16) |
| Sn2—N2—C2—S2 | 174.6 (3) | C42—C43—C44—F6 | −178.9 (9) |
| C1—S2—C2—N2 | −0.5 (6) | C43—C44—C45—C46 | −0.6 (16) |
| C1—S2—C2—S3 | −179.7 (6) | F6—C44—C45—C46 | 178.6 (9) |
| O1—Sn2—C5—C6 | −29.7 (7) | C44—C45—C46—C41 | −0.3 (15) |
| C12—Sn2—C5—C6 | 157.5 (5) | C42—C41—C46—C45 | 1.5 (12) |
| O2—Sn2—C5—C6 | −100.2 (6) | C40—C41—C46—C45 | 180.0 (8) |
| N2—Sn2—C5—C6 | 53.1 (6) | C49$^{i}$—C47—C48—C49 | −0.1 (15) |
| Sn2—C5—C6—C11 | 97.7 (8) | C47—C48—C49—C47$^{i}$ | 0.1 (15) |

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1.

**Fig. 1**

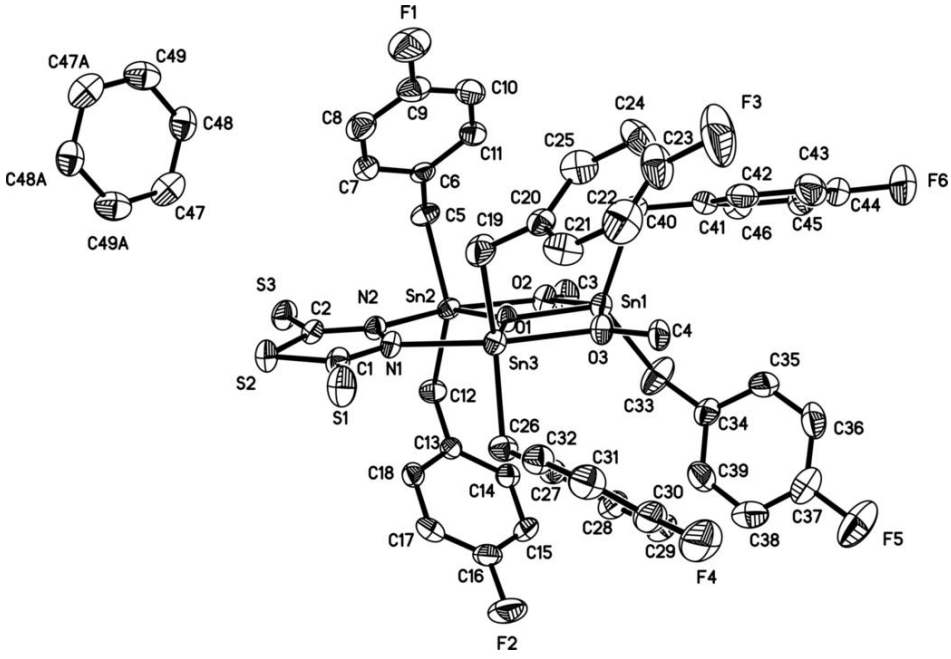
F1
C47A
C49
C10
C24
F3
C48
C8
C9
C23
C25
C43
C48A
C11
C42
F6
C7
C6
C20
C22
C44
C47
C5
C19
C21
C40
C41
C46
C45
C49A
S3
O2
C3
C2
N2
Sn2
Sn1
O1
C4
C1
N1
Sn3
O3
C35
S2
C12
C33
S1
C26
C32
C34
C36
C13
C31
C18
C14
C27
C30
C39
C28
C37
C17
C15
C29
C38
F5
C16
F4
F2

**Fig. 2**