

[μ -2,2'-Dimethyl-2,2'-(*p*-phenylene)-dipropyl]bis[chloridobis(2-methyl-2-phenylpropyl)tin(IV)]

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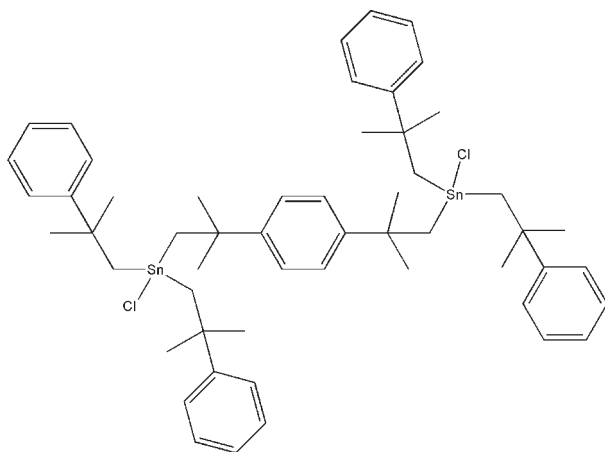
Received 14 March 2010; accepted 28 March 2010

Key indicators: single-crystal X-ray study; $T = 185$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.056; wR factor = 0.113; data-to-parameter ratio = 19.0.

The molecular structure of the title compound, $[\text{Sn}_2(\text{C}_{10}\text{H}_{13})_4(\text{C}_{14}\text{H}_{20})\text{Cl}_2]$, is a binuclear centrosymmetric complex, in which the Sn atoms are four-coordinated by three C atoms and one Cl atom in a distorted tetrahedral geometry.

Related literature

For general background to organotin compounds, see: Chandrasekhar *et al.* (2002); Wu *et al.* (2009); For related structures, see: Tarassoli *et al.* (2002).



Experimental

Crystal data

$[\text{Sn}_2(\text{C}_{10}\text{H}_{13})_4(\text{C}_{14}\text{H}_{20})\text{Cl}_2]$
 $M_r = 1029.40$
 Monoclinic, $C2/c$
 $a = 15.0769$ (19) Å
 $b = 17.773$ (2) Å
 $c = 18.914$ (2) Å
 $\beta = 94.674$ (2)°
 $V = 5051.4$ (11) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.13$ mm⁻¹
 $T = 185$ K
 $0.34 \times 0.32 \times 0.29$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.688$, $T_{\max} = 0.721$
 14065 measured reflections
 4976 independent reflections
 3284 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.073$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.056$
 $wR(F^2) = 0.113$
 $S = 1.02$
 4976 reflections
 262 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.78$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.42$ e Å⁻³

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL-Plus (Sheldrick, 2008); software used to prepare material for publication: SHELXTL-Plus.

We thank the State Key Development Program for Basic Research of China (2005CB221304) for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PB2026).

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 Tarassoli, A., Asadi, A. & Hitchcock, P. B. (2002). *J. Organomet. Chem.* **645**, 105–111.
 Wu, X., Kang, W., Zhu, D., Zhu, C. & Liu, S. (2009). *J. Organomet. Chem.* **694**, 2981–2986.

supplementary materials

Acta Cryst. (2010). E66, m495 [doi:10.1107/S1600536810011670]

[μ -2,2'-Dimethyl-2,2'-(*p*-phenylene)dipropyl]bis[chloridobis(2-methyl-2-phenylpropyl)tin(IV)]

C. Sun, C. Liang, W. Kang and D. Zhu

Comment

The increasing interest in organotin compounds that has arisen in the last few decades is attributed to their significantly important biological properties like antiviral and anticancer agents, in vitro antibacterial and antifungal agents, wood preservatives and pesticides, etc. (Chandrasekhar *et al.*, 2002; & Wu *et al.*, 2009). Therefore, synthesis of new organotin compounds with different structural features will be beneficial in the development of pharmaceutical organotin and in other properties and application. herein, we present the synthesis and crystal structure of the title compound (I).

The structure of the title compound (Fig.1) consists of two symmetry equivalent tin moieties, where the tin atoms are tetrahedrally coordinated by the three C atoms and one Cl atom. The bond lengths for Sn(1)—C(1), Sn(1)—C(8) and Sn(1)—C(18) are 2.146 (5), 2.152 (5) and 2.149 (5) Å, respectively, which are slightly shorter than the Bz₃Sn(EtACDA) reported by Tarassoli *et al.* (Tarassoli *et al.*, 2002). Around the tin, the angles C(1)—Sn(1)—C(8), C(1)—Sn(1)—C(18) and C(8)—Sn(1)—C(18) are wider while the C(1)—Sn(1)—Cl(1), C(8)—Sn(1)—Cl(1) and C(18)—Sn(1)—Cl(1) are narrower than the ideal tetrahedral angle. Thus, the environment of tin is best described as distorted tetrahedral.

Experimental

A small iodine grain, magnesium powder(0.24 g 10 mmol), and 1,4-bis(1-chloro-2-methylpropan-2-yl)benzene (0.52 g, 2 mmol) were added to 2 ml of anhydrous ether under stirring. The reaction mixture is then heated to 50–60°C by hot-water bath and maintained slight boiling state. When the purplish red of iodine disappeared, which indicated the reaction were initiated, the hot-water bath was removed. The reaction were keeping the slight boiling state, then a solution of 1,4-bis(1-chloro-2-methylpropan-2-yl)benzene (2.59 g, 10 mmol) in 10 ml anhydrous ether were added dropwise. After finished, the mixture was refluxed for 1 h to allow magnesium to proceed to completion, then cooled to 0–5°C by ice-salt bath. A solution of dichlorobis(2-methyl-2-phenylpropyl)stannane (4.56 g, 10 mmol) in 15 mL THF were then added dropwise. After finished, the ice-salt bath was removed, and the reaction mixture were stirred for 0.5 h at room temprature then refluxed for another 1.5 h. Finally, the mixture were again cooled to 0°C, and acidified by dropwise adding a solution containing 2.5 g fuming HCl and 15 ml water. The layers were separated, the organic phase was dried over anhydrous calcium chloride. Following filtration and evaporation of the solvent, the residue was recrystallized by THF and the colorless block crystals of (I) were obtained.

Refinement

All H atoms on C atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{carrier})$.

Figures

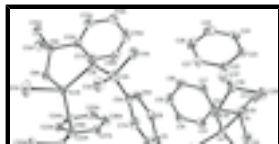


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids. H atoms have been omitted for clarity. Scheme 1. The chemical structure diagram of (I). Scheme 2. The reaction scheme for synthesis of (I).

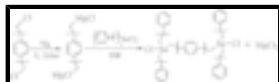


Fig. 2. The formation of the title compound.

[μ -2,2'-Dimethyl-2,2'-(*p*-phenylene)dipropyl]bis[chloridobis(2-methyl-2-phenylpropyl)tin(IV)]

Crystal data

| | |
|--|---|
| $[\text{Sn}_2(\text{C}_{10}\text{H}_{13})_4(\text{C}_{14}\text{H}_{20})\text{Cl}_2]$ | $F(000) = 2120$ |
| $M_r = 1029.40$ | $D_x = 1.354 \text{ Mg m}^{-3}$ |
| Monoclinic, $C2/c$ | Melting point: not measured K |
| Hall symbol: $-C 2yc$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| $a = 15.0769 (19) \text{ \AA}$ | Cell parameters from 4976 reflections |
| $b = 17.773 (2) \text{ \AA}$ | $\theta = 1.8\text{--}26.1^\circ$ |
| $c = 18.914 (2) \text{ \AA}$ | $\mu = 1.13 \text{ mm}^{-1}$ |
| $\beta = 94.674 (2)^\circ$ | $T = 185 \text{ K}$ |
| $V = 5051.4 (11) \text{ \AA}^3$ | Block, colorless |
| $Z = 4$ | $0.34 \times 0.32 \times 0.29 \text{ mm}$ |

Data collection

| | |
|---|--|
| Bruker SMART APEX CCD area-detector diffractometer | 4976 independent reflections |
| Radiation source: fine-focus sealed tube graphite | 3284 reflections with $I > 2\sigma(I)$ |
| phi and ω scans | $R_{\text{int}} = 0.073$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $\theta_{\text{max}} = 26.1^\circ$, $\theta_{\text{min}} = 1.8^\circ$ |
| $T_{\text{min}} = 0.688$, $T_{\text{max}} = 0.721$ | $h = -17 \rightarrow 18$ |
| 14065 measured reflections | $k = -21 \rightarrow 10$ |
| | $l = -22 \rightarrow 23$ |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.056$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.113$ | H-atom parameters constrained |
| $S = 1.02$ | $w = 1/[\sigma^2(F_o^2) + (0.039P)^2]$ |
| | where $P = (F_o^2 + 2F_c^2)/3$ |

| | |
|------------------|--|
| 4976 reflections | $(\Delta/\sigma)_{\max} = 0.001$ |
| 262 parameters | $\Delta\rho_{\max} = 0.78 \text{ e } \text{\AA}^{-3}$ |
| 0 restraints | $\Delta\rho_{\min} = -0.42 \text{ e } \text{\AA}^{-3}$ |

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.

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|--------------|--------------|----------------------------------|
| Sn1 | 0.28085 (2) | 0.63191 (2) | 0.82050 (2) | 0.03363 (14) |
| Cl1 | 0.38105 (10) | 0.72044 (11) | 0.88005 (10) | 0.0654 (6) |
| C1 | 0.1798 (3) | 0.6193 (4) | 0.8932 (3) | 0.0452 (17) |
| H1A | 0.1553 | 0.5691 | 0.8870 | 0.054* |
| H1B | 0.2087 | 0.6218 | 0.9409 | 0.054* |
| C2 | 0.1012 (3) | 0.6751 (3) | 0.8892 (3) | 0.0379 (15) |
| C3 | 0.1392 (4) | 0.7525 (4) | 0.9106 (3) | 0.0584 (19) |
| H3A | 0.0919 | 0.7887 | 0.9090 | 0.088* |
| H3B | 0.1819 | 0.7672 | 0.8782 | 0.088* |
| H3C | 0.1677 | 0.7500 | 0.9578 | 0.088* |
| C4 | 0.0385 (4) | 0.6530 (4) | 0.9459 (3) | 0.0521 (19) |
| H4A | -0.0105 | 0.6877 | 0.9445 | 0.078* |
| H4B | 0.0703 | 0.6546 | 0.9919 | 0.078* |
| H4C | 0.0163 | 0.6031 | 0.9366 | 0.078* |
| C5 | 0.0505 (3) | 0.6738 (4) | 0.8170 (3) | 0.0362 (14) |
| C6 | 0.0253 (4) | 0.6067 (4) | 0.7834 (3) | 0.0442 (16) |
| H6A | 0.0417 | 0.5612 | 0.8050 | 0.053* |
| C7 | 0.0247 (4) | 0.7404 (4) | 0.7826 (3) | 0.0476 (17) |
| H7A | 0.0411 | 0.7861 | 0.8038 | 0.057* |
| C8 | 0.3641 (3) | 0.5345 (3) | 0.8122 (3) | 0.0376 (15) |
| H8A | 0.3510 | 0.5132 | 0.7653 | 0.045* |
| H8B | 0.4254 | 0.5516 | 0.8150 | 0.045* |
| C9 | 0.3579 (3) | 0.4711 (4) | 0.8663 (3) | 0.0394 (15) |
| C10 | 0.3954 (4) | 0.4993 (4) | 0.9392 (3) | 0.062 (2) |
| H10A | 0.3599 | 0.5405 | 0.9537 | 0.093* |
| H10B | 0.4556 | 0.5159 | 0.9364 | 0.093* |
| H10C | 0.3942 | 0.4593 | 0.9731 | 0.093* |
| C11 | 0.4168 (4) | 0.4049 (4) | 0.8449 (4) | 0.060 (2) |
| H11A | 0.4772 | 0.4217 | 0.8439 | 0.090* |

supplementary materials

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|------|------------|------------|------------|-------------|
| H11B | 0.3955 | 0.3869 | 0.7988 | 0.090* |
| H11C | 0.4143 | 0.3649 | 0.8789 | 0.090* |
| C12 | 0.2626 (3) | 0.4417 (3) | 0.8674 (3) | 0.0350 (14) |
| C13 | 0.2205 (4) | 0.4316 (3) | 0.9293 (3) | 0.0434 (16) |
| H13A | 0.2508 | 0.4431 | 0.9727 | 0.052* |
| C14 | 0.1342 (4) | 0.4048 (3) | 0.9273 (4) | 0.0462 (16) |
| H14A | 0.1073 | 0.3984 | 0.9694 | 0.055* |
| C15 | 0.0884 (4) | 0.3878 (4) | 0.8646 (4) | 0.0567 (19) |
| H15A | 0.0304 | 0.3698 | 0.8639 | 0.068* |
| C16 | 0.1283 (4) | 0.3974 (4) | 0.8018 (4) | 0.0570 (19) |
| H16A | 0.0974 | 0.3861 | 0.7585 | 0.068* |
| C17 | 0.2147 (4) | 0.4239 (4) | 0.8044 (3) | 0.0474 (17) |
| H17A | 0.2414 | 0.4300 | 0.7622 | 0.057* |
| C18 | 0.2457 (3) | 0.6893 (3) | 0.7222 (3) | 0.0373 (14) |
| H18A | 0.1817 | 0.6855 | 0.7121 | 0.045* |
| H18B | 0.2596 | 0.7422 | 0.7291 | 0.045* |
| C19 | 0.2896 (4) | 0.6625 (3) | 0.6566 (3) | 0.0355 (14) |
| C20 | 0.3905 (4) | 0.6750 (4) | 0.6689 (3) | 0.0496 (17) |
| H20A | 0.4140 | 0.6446 | 0.7081 | 0.074* |
| H20B | 0.4022 | 0.7270 | 0.6794 | 0.074* |
| H20C | 0.4185 | 0.6611 | 0.6270 | 0.074* |
| C21 | 0.2556 (4) | 0.7128 (3) | 0.5935 (3) | 0.0483 (17) |
| H21A | 0.1925 | 0.7063 | 0.5843 | 0.072* |
| H21B | 0.2848 | 0.6988 | 0.5522 | 0.072* |
| H21C | 0.2683 | 0.7645 | 0.6049 | 0.072* |
| C22 | 0.2664 (3) | 0.5811 (3) | 0.6383 (3) | 0.0332 (14) |
| C23 | 0.3288 (4) | 0.5275 (4) | 0.6238 (3) | 0.0404 (15) |
| H23A | 0.3885 | 0.5412 | 0.6259 | 0.048* |
| C24 | 0.3056 (5) | 0.4547 (4) | 0.6065 (3) | 0.0501 (17) |
| H24A | 0.3496 | 0.4204 | 0.5969 | 0.060* |
| C25 | 0.2180 (5) | 0.4319 (4) | 0.6032 (3) | 0.0541 (18) |
| H25A | 0.2023 | 0.3825 | 0.5918 | 0.065* |
| C26 | 0.1550 (4) | 0.4837 (4) | 0.6171 (3) | 0.0500 (17) |
| H26A | 0.0956 | 0.4693 | 0.6153 | 0.060* |
| C27 | 0.1778 (4) | 0.5575 (4) | 0.6339 (3) | 0.0412 (15) |
| H27A | 0.1334 | 0.5919 | 0.6424 | 0.049* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|-------------|-------------|-------------|--------------|--------------|
| Sn1 | 0.0262 (2) | 0.0405 (2) | 0.0342 (2) | 0.0021 (2) | 0.00262 (15) | -0.0040 (2) |
| C11 | 0.0347 (8) | 0.0812 (14) | 0.0794 (13) | -0.0075 (9) | -0.0002 (8) | -0.0371 (11) |
| C1 | 0.030 (3) | 0.072 (5) | 0.033 (3) | 0.003 (3) | 0.004 (2) | 0.008 (3) |
| C2 | 0.027 (3) | 0.037 (4) | 0.050 (4) | 0.001 (3) | 0.003 (3) | -0.007 (3) |
| C3 | 0.042 (4) | 0.074 (5) | 0.059 (4) | -0.004 (4) | 0.002 (3) | -0.017 (4) |
| C4 | 0.033 (3) | 0.083 (6) | 0.041 (4) | -0.003 (3) | 0.007 (3) | -0.006 (4) |
| C5 | 0.023 (3) | 0.047 (4) | 0.040 (3) | 0.007 (3) | 0.009 (2) | 0.002 (3) |
| C6 | 0.039 (4) | 0.049 (4) | 0.047 (4) | 0.001 (3) | 0.014 (3) | 0.005 (3) |

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|-----|-----------|-----------|-----------|------------|------------|------------|
| C7 | 0.039 (4) | 0.048 (4) | 0.056 (4) | 0.006 (3) | 0.003 (3) | -0.001 (3) |
| C8 | 0.032 (3) | 0.048 (4) | 0.035 (3) | 0.003 (3) | 0.010 (3) | -0.002 (3) |
| C9 | 0.033 (3) | 0.054 (4) | 0.032 (3) | 0.009 (3) | 0.007 (3) | 0.011 (3) |
| C10 | 0.047 (4) | 0.094 (6) | 0.044 (4) | -0.005 (4) | -0.009 (3) | 0.009 (4) |
| C11 | 0.044 (4) | 0.057 (5) | 0.079 (5) | 0.026 (4) | 0.009 (4) | 0.020 (4) |
| C12 | 0.031 (3) | 0.033 (4) | 0.041 (4) | 0.007 (3) | 0.003 (3) | 0.002 (3) |
| C13 | 0.050 (4) | 0.039 (4) | 0.042 (4) | 0.010 (3) | 0.007 (3) | 0.002 (3) |
| C14 | 0.047 (4) | 0.039 (4) | 0.055 (4) | 0.003 (3) | 0.018 (3) | 0.005 (3) |
| C15 | 0.037 (4) | 0.039 (4) | 0.093 (6) | -0.002 (3) | 0.005 (4) | -0.002 (4) |
| C16 | 0.054 (4) | 0.062 (5) | 0.053 (4) | 0.009 (4) | -0.010 (3) | -0.008 (4) |
| C17 | 0.045 (4) | 0.052 (4) | 0.044 (4) | 0.011 (3) | 0.003 (3) | 0.003 (3) |
| C18 | 0.033 (3) | 0.033 (3) | 0.046 (4) | -0.003 (3) | 0.003 (3) | -0.002 (3) |
| C19 | 0.035 (3) | 0.037 (4) | 0.036 (3) | 0.002 (3) | 0.006 (3) | 0.008 (3) |
| C20 | 0.042 (4) | 0.047 (4) | 0.061 (4) | -0.011 (3) | 0.013 (3) | 0.004 (4) |
| C21 | 0.052 (4) | 0.044 (4) | 0.049 (4) | -0.001 (3) | 0.005 (3) | 0.009 (3) |
| C22 | 0.032 (3) | 0.043 (4) | 0.025 (3) | 0.003 (3) | 0.003 (2) | 0.002 (3) |
| C23 | 0.038 (3) | 0.049 (4) | 0.034 (3) | 0.004 (3) | 0.002 (3) | -0.001 (3) |
| C24 | 0.064 (4) | 0.047 (4) | 0.039 (4) | 0.010 (4) | 0.003 (3) | -0.009 (3) |
| C25 | 0.089 (5) | 0.032 (4) | 0.040 (4) | -0.005 (4) | -0.001 (4) | -0.002 (3) |
| C26 | 0.045 (4) | 0.048 (4) | 0.057 (4) | -0.020 (4) | 0.002 (3) | 0.004 (4) |
| C27 | 0.032 (3) | 0.043 (4) | 0.049 (4) | 0.003 (3) | 0.007 (3) | 0.006 (3) |

Geometric parameters (Å, °)

| | | | |
|--------------------|-------------|----------|-----------|
| Sn1—C1 | 2.146 (5) | C12—C17 | 1.378 (7) |
| Sn1—C18 | 2.149 (5) | C12—C13 | 1.387 (7) |
| Sn1—C8 | 2.152 (5) | C13—C14 | 1.384 (8) |
| Sn1—C11 | 2.3978 (17) | C13—H13A | 0.9300 |
| C1—C2 | 1.541 (7) | C14—C15 | 1.356 (8) |
| C1—H1A | 0.9700 | C14—H14A | 0.9300 |
| C1—H1B | 0.9700 | C15—C16 | 1.386 (9) |
| C2—C5 | 1.511 (7) | C15—H15A | 0.9300 |
| C2—C3 | 1.532 (8) | C16—C17 | 1.382 (8) |
| C2—C4 | 1.537 (7) | C16—H16A | 0.9300 |
| C3—H3A | 0.9600 | C17—H17A | 0.9300 |
| C3—H3B | 0.9600 | C18—C19 | 1.529 (7) |
| C3—H3C | 0.9600 | C18—H18A | 0.9700 |
| C4—H4A | 0.9600 | C18—H18B | 0.9700 |
| C4—H4B | 0.9600 | C19—C22 | 1.522 (8) |
| C4—H4C | 0.9600 | C19—C20 | 1.536 (7) |
| C5—C6 | 1.389 (8) | C19—C21 | 1.545 (7) |
| C5—C7 | 1.391 (8) | C20—H20A | 0.9600 |
| C6—C6 ⁱ | 1.422 (11) | C20—H20B | 0.9600 |
| C6—H6A | 0.9300 | C20—H20C | 0.9600 |
| C7—C7 ⁱ | 1.387 (11) | C21—H21A | 0.9600 |
| C7—H7A | 0.9300 | C21—H21B | 0.9600 |
| C8—C9 | 1.530 (7) | C21—H21C | 0.9600 |
| C8—H8A | 0.9700 | C22—C23 | 1.382 (7) |
| C8—H8B | 0.9700 | C22—C27 | 1.395 (7) |

supplementary materials

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|-------------------------|-------------|---------------|-----------|
| C9—C12 | 1.531 (7) | C23—C24 | 1.373 (8) |
| C9—C10 | 1.531 (8) | C23—H23A | 0.9300 |
| C9—C11 | 1.548 (8) | C24—C25 | 1.378 (8) |
| C10—H10A | 0.9600 | C24—H24A | 0.9300 |
| C10—H10B | 0.9600 | C25—C26 | 1.365 (8) |
| C10—H10C | 0.9600 | C25—H25A | 0.9300 |
| C11—H11A | 0.9600 | C26—C27 | 1.386 (8) |
| C11—H11B | 0.9600 | C26—H26A | 0.9300 |
| C11—H11C | 0.9600 | C27—H27A | 0.9300 |
| C1—Sn1—C18 | 117.8 (2) | H11B—C11—H11C | 109.5 |
| C1—Sn1—C8 | 114.3 (2) | C17—C12—C13 | 117.1 (5) |
| C18—Sn1—C8 | 115.0 (2) | C17—C12—C9 | 119.5 (5) |
| C1—Sn1—C11 | 102.73 (17) | C13—C12—C9 | 123.4 (5) |
| C18—Sn1—C11 | 101.32 (16) | C14—C13—C12 | 121.0 (6) |
| C8—Sn1—C11 | 102.30 (16) | C14—C13—H13A | 119.5 |
| C2—C1—Sn1 | 119.0 (4) | C12—C13—H13A | 119.5 |
| C2—C1—H1A | 107.6 | C15—C14—C13 | 120.8 (6) |
| Sn1—C1—H1A | 107.6 | C15—C14—H14A | 119.6 |
| C2—C1—H1B | 107.6 | C13—C14—H14A | 119.6 |
| Sn1—C1—H1B | 107.6 | C14—C15—C16 | 119.7 (6) |
| H1A—C1—H1B | 107.0 | C14—C15—H15A | 120.1 |
| C5—C2—C3 | 113.7 (5) | C16—C15—H15A | 120.1 |
| C5—C2—C4 | 109.4 (4) | C17—C16—C15 | 119.0 (6) |
| C3—C2—C4 | 106.5 (5) | C17—C16—H16A | 120.5 |
| C5—C2—C1 | 111.4 (5) | C15—C16—H16A | 120.5 |
| C3—C2—C1 | 107.2 (5) | C12—C17—C16 | 122.3 (6) |
| C4—C2—C1 | 108.4 (5) | C12—C17—H17A | 118.8 |
| C2—C3—H3A | 109.5 | C16—C17—H17A | 118.8 |
| C2—C3—H3B | 109.5 | C19—C18—Sn1 | 117.4 (4) |
| H3A—C3—H3B | 109.5 | C19—C18—H18A | 107.9 |
| C2—C3—H3C | 109.5 | Sn1—C18—H18A | 107.9 |
| H3A—C3—H3C | 109.5 | C19—C18—H18B | 107.9 |
| H3B—C3—H3C | 109.5 | Sn1—C18—H18B | 107.9 |
| C2—C4—H4A | 109.5 | H18A—C18—H18B | 107.2 |
| C2—C4—H4B | 109.5 | C22—C19—C18 | 112.0 (4) |
| H4A—C4—H4B | 109.5 | C22—C19—C20 | 112.2 (5) |
| C2—C4—H4C | 109.5 | C18—C19—C20 | 108.8 (5) |
| H4A—C4—H4C | 109.5 | C22—C19—C21 | 108.5 (5) |
| H4B—C4—H4C | 109.5 | C18—C19—C21 | 107.9 (5) |
| C6—C5—C7 | 117.5 (5) | C20—C19—C21 | 107.2 (5) |
| C6—C5—C2 | 121.7 (5) | C19—C20—H20A | 109.5 |
| C7—C5—C2 | 120.8 (6) | C19—C20—H20B | 109.5 |
| C5—C6—C6 ⁱ | 120.9 (3) | H20A—C20—H20B | 109.5 |
| C5—C6—H6A | 119.6 | C19—C20—H20C | 109.5 |
| C6 ⁱ —C6—H6A | 119.6 | H20A—C20—H20C | 109.5 |
| C7 ⁱ —C7—C5 | 121.7 (4) | H20B—C20—H20C | 109.5 |
| C7 ⁱ —C7—H7A | 119.2 | C19—C21—H21A | 109.5 |
| C5—C7—H7A | 119.2 | C19—C21—H21B | 109.5 |

| | | | |
|--------------------------|------------|-----------------|------------|
| C9—C8—Sn1 | 118.4 (3) | H21A—C21—H21B | 109.5 |
| C9—C8—H8A | 107.7 | C19—C21—H21C | 109.5 |
| Sn1—C8—H8A | 107.7 | H21A—C21—H21C | 109.5 |
| C9—C8—H8B | 107.7 | H21B—C21—H21C | 109.5 |
| Sn1—C8—H8B | 107.7 | C23—C22—C27 | 116.4 (6) |
| H8A—C8—H8B | 107.1 | C23—C22—C19 | 123.5 (5) |
| C8—C9—C12 | 111.7 (5) | C27—C22—C19 | 120.0 (5) |
| C8—C9—C10 | 108.8 (5) | C24—C23—C22 | 122.2 (6) |
| C12—C9—C10 | 112.2 (5) | C24—C23—H23A | 118.9 |
| C8—C9—C11 | 108.5 (4) | C22—C23—H23A | 118.9 |
| C12—C9—C11 | 107.6 (5) | C23—C24—C25 | 120.9 (6) |
| C10—C9—C11 | 107.8 (5) | C23—C24—H24A | 119.6 |
| C9—C10—H10A | 109.5 | C25—C24—H24A | 119.6 |
| C9—C10—H10B | 109.5 | C26—C25—C24 | 118.1 (6) |
| H10A—C10—H10B | 109.5 | C26—C25—H25A | 120.9 |
| C9—C10—H10C | 109.5 | C24—C25—H25A | 120.9 |
| H10A—C10—H10C | 109.5 | C25—C26—C27 | 121.3 (6) |
| H10B—C10—H10C | 109.5 | C25—C26—H26A | 119.4 |
| C9—C11—H11A | 109.5 | C27—C26—H26A | 119.4 |
| C9—C11—H11B | 109.5 | C26—C27—C22 | 121.1 (6) |
| H11A—C11—H11B | 109.5 | C26—C27—H27A | 119.5 |
| C9—C11—H11C | 109.5 | C22—C27—H27A | 119.5 |
| H11A—C11—H11C | 109.5 | | |
| C18—Sn1—C1—C2 | -23.9 (5) | C17—C12—C13—C14 | 0.0 (9) |
| C8—Sn1—C1—C2 | -163.6 (4) | C9—C12—C13—C14 | -180.0 (5) |
| C11—Sn1—C1—C2 | 86.4 (4) | C12—C13—C14—C15 | -0.1 (9) |
| Sn1—C1—C2—C5 | 58.8 (6) | C13—C14—C15—C16 | -0.1 (10) |
| Sn1—C1—C2—C3 | -66.2 (6) | C14—C15—C16—C17 | 0.3 (10) |
| Sn1—C1—C2—C4 | 179.2 (4) | C13—C12—C17—C16 | 0.2 (9) |
| C3—C2—C5—C6 | 168.2 (5) | C9—C12—C17—C16 | -179.8 (6) |
| C4—C2—C5—C6 | -72.9 (7) | C15—C16—C17—C12 | -0.4 (10) |
| C1—C2—C5—C6 | 46.9 (7) | C1—Sn1—C18—C19 | -145.8 (4) |
| C3—C2—C5—C7 | -13.9 (7) | C8—Sn1—C18—C19 | -6.4 (5) |
| C4—C2—C5—C7 | 105.0 (6) | C11—Sn1—C18—C19 | 103.1 (4) |
| C1—C2—C5—C7 | -135.2 (5) | Sn1—C18—C19—C22 | 61.7 (5) |
| C7—C5—C6—C6 ⁱ | -0.3 (10) | Sn1—C18—C19—C20 | -62.9 (6) |
| C2—C5—C6—C6 ⁱ | 177.7 (6) | Sn1—C18—C19—C21 | -179.0 (4) |
| C6—C5—C7—C7 ⁱ | 0.4 (10) | C18—C19—C22—C23 | -131.9 (5) |
| C2—C5—C7—C7 ⁱ | -177.6 (6) | C20—C19—C22—C23 | -9.2 (7) |
| C1—Sn1—C8—C9 | -11.0 (5) | C21—C19—C22—C23 | 109.1 (6) |
| C18—Sn1—C8—C9 | -151.8 (4) | C18—C19—C22—C27 | 49.5 (7) |
| C11—Sn1—C8—C9 | 99.3 (4) | C20—C19—C22—C27 | 172.2 (5) |
| Sn1—C8—C9—C12 | 56.1 (6) | C21—C19—C22—C27 | -69.5 (6) |
| Sn1—C8—C9—C10 | -68.3 (5) | C27—C22—C23—C24 | -0.5 (8) |
| Sn1—C8—C9—C11 | 174.6 (4) | C19—C22—C23—C24 | -179.1 (5) |
| C8—C9—C12—C17 | 48.6 (7) | C22—C23—C24—C25 | -0.3 (9) |
| C10—C9—C12—C17 | 171.1 (6) | C23—C24—C25—C26 | 0.4 (9) |
| C11—C9—C12—C17 | -70.4 (7) | C24—C25—C26—C27 | 0.3 (9) |

supplementary materials

| | | | |
|----------------|------------|-----------------|-----------|
| C8—C9—C12—C13 | -131.4 (6) | C25—C26—C27—C22 | -1.1 (9) |
| C10—C9—C12—C13 | -8.9 (8) | C23—C22—C27—C26 | 1.1 (8) |
| C11—C9—C12—C13 | 109.6 (6) | C19—C22—C27—C26 | 179.8 (5) |

Symmetry codes: (i) $-x, y, -z+3/2$.

Fig. 1

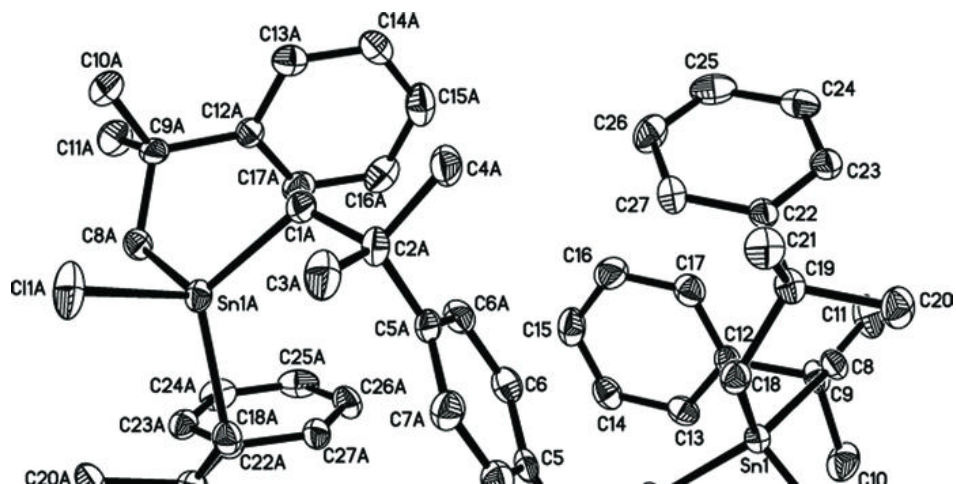


Fig. 2

