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Tricyclohexyl(2,3-dibromo-3-phenylpropionato- κ O)tin(IV)

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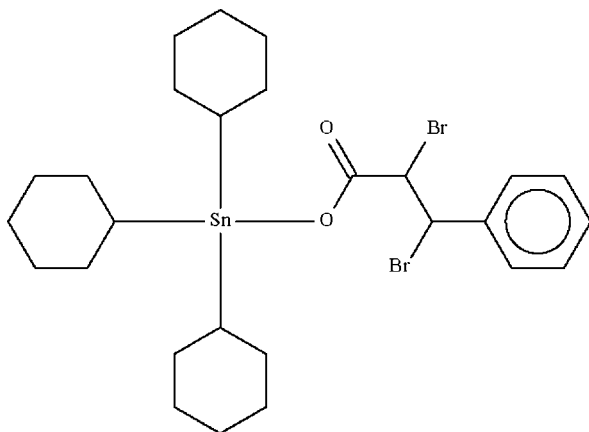
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Key indicators: single-crystal X-ray study; $T = 118$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å;
 R factor = 0.032; wR factor = 0.083; data-to-parameter ratio = 21.9.

Tricyclohexyltin cinnamate reacts with 4,4-dimethylamino-pyridine hydrobromide perbromide to form the title compound, $[\text{Sn}(\text{C}_6\text{H}_{11})_3(\text{C}_9\text{H}_7\text{Br}_2\text{O}_2)]$, which exists as a monomeric molecule with the Sn atom in a distorted tetrahedral C_3O coordination geometry.

Related literature

For reviews of the structural chemistry of organotin carboxylates, see: Tiekink (1991, 1994).



Experimental

Crystal data

$[\text{Sn}(\text{C}_6\text{H}_{11})_3(\text{C}_9\text{H}_7\text{Br}_2\text{O}_2)]$
 $M_r = 675.10$
Monoclinic, $P2_1/c$
 $a = 21.2359$ (3) Å
 $b = 9.0837$ (1) Å
 $c = 15.0550$ (2) Å
 $\beta = 108.287$ (1)°

$V = 2757.45$ (6) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 3.85$ mm⁻¹
 $T = 118$ K
 $0.30 \times 0.20 \times 0.10$ mm

Data collection

Bruker SMART APEX
diffractometer
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.392$, $T_{\max} = 0.700$

21967 measured reflections
6325 independent reflections
5007 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.083$
 $S = 1.04$
6325 reflections

289 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.63$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.13$ e Å⁻³

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the University of Malaya (FS339/2008 A) for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2413).

References

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supplementary materials

Acta Cryst. (2009). E65, m490 [doi:10.1107/S1600536809012240]

Tricyclohexyl(2,3-dibromo-3-phenylpropionato- κO)tin(IV)

P. Y. Thong, K. M. Lo and S. W. Ng

Comment

(type here to add)

Experimental

Tricyclohexyltin chloride (1.93 g, 5 mmol) was reacted with cinnamic acid (0.74 g, 5 mmol) in ethanol (100 ml) under reflux for 2 h. The product, tricyclohexyltin cinnamate, was collected upon removal of the solvent. The organotin compound (1 g, 2 mmol) and 4,4-dimethylaminopyridine hydrobromide perbromide (0.73 g, 2 mmol) were heated in 1:1 ethanol:chloroform (100 ml) for 1 h. Slow evaporation of the filtrate gave colorless crystals.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.95 to 1.00 Å) and were included in the refinement in the riding model approximation, with $U(H)$ set to $1.2U(C)$. The large peak/hole is in the vicinity (about 1 Å) of the C21 atom.

Figures

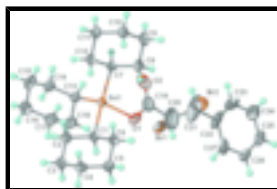


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $\text{Sn}(\text{C}_6\text{H}_{11})_3(\text{C}_9\text{H}_7\text{Br}_2\text{O}_2)$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

Tricyclohexyl(2,3-dibromo-3-phenylpropionato- κO)tin(IV)

Crystal data

$[\text{Sn}(\text{C}_6\text{H}_{11})_3(\text{C}_9\text{H}_7\text{Br}_2\text{O}_2)]$

$M_r = 675.10$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 21.2359$ (3) Å

$b = 9.0837$ (1) Å

$c = 15.0550$ (2) Å

$\beta = 108.287$ (1)°

$V = 2757.45$ (6) Å³

$Z = 4$

$F_{000} = 1352$

$D_x = 1.626$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 7301 reflections

$\theta = 2.5\text{--}28.2^\circ$

$\mu = 3.85$ mm⁻¹

$T = 118$ K

Block, colorless

$0.30 \times 0.20 \times 0.10$ mm

supplementary materials

Data collection

| | |
|---|--|
| Bruker SMART APEX diffractometer | 6325 independent reflections |
| Radiation source: fine-focus sealed tube | 5007 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.034$ |
| $T = 118$ K | $\theta_{\text{max}} = 27.5^\circ$ |
| ω scans | $\theta_{\text{min}} = 1.0^\circ$ |
| Absorption correction: Multi-scan (SADABS; Sheldrick, 1996) | $h = -27 \rightarrow 27$ |
| $T_{\text{min}} = 0.392$, $T_{\text{max}} = 0.700$ | $k = -11 \rightarrow 11$ |
| 21967 measured reflections | $l = -18 \rightarrow 19$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.032$ | H-atom parameters constrained |
| $wR(F^2) = 0.083$ | $w = 1/[\sigma^2(F_o^2) + (0.0318P)^2 + 6.5266P]$ |
| $S = 1.04$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 6325 reflections | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| 289 parameters | $\Delta\rho_{\text{max}} = 1.63 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\text{min}} = -1.13 \text{ e } \text{\AA}^{-3}$ |
| | Extinction correction: none |

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|-------------|---------------|----------------------------------|
| Sn1 | 0.213693 (12) | 0.54260 (3) | 0.484115 (16) | 0.02051 (7) |
| Br1 | 0.43779 (2) | 0.37225 (5) | 0.44008 (3) | 0.03484 (11) |
| Br2 | 0.258387 (19) | 0.05999 (4) | 0.32990 (3) | 0.03129 (10) |
| O1 | 0.26589 (15) | 0.4358 (3) | 0.4077 (2) | 0.0387 (7) |
| O2 | 0.31430 (15) | 0.2973 (3) | 0.5299 (2) | 0.0452 (8) |
| C1 | 0.15692 (17) | 0.6666 (4) | 0.3632 (2) | 0.0220 (7) |
| H1 | 0.1895 | 0.7061 | 0.3336 | 0.026* |
| C2 | 0.12163 (19) | 0.7996 (4) | 0.3873 (3) | 0.0264 (8) |
| H2A | 0.0894 | 0.7659 | 0.4183 | 0.032* |
| H2B | 0.1545 | 0.8636 | 0.4318 | 0.032* |
| C3 | 0.08542 (19) | 0.8880 (4) | 0.3002 (3) | 0.0279 (8) |
| H3A | 0.0604 | 0.9690 | 0.3177 | 0.033* |
| H3B | 0.1183 | 0.9324 | 0.2739 | 0.033* |
| C4 | 0.03775 (18) | 0.7926 (4) | 0.2262 (3) | 0.0275 (8) |
| H4A | 0.0178 | 0.8519 | 0.1691 | 0.033* |
| H4B | 0.0015 | 0.7587 | 0.2494 | 0.033* |
| C5 | 0.07263 (19) | 0.6598 (4) | 0.2018 (2) | 0.0282 (8) |

| | | | | |
|------|--------------|-------------|------------|-------------|
| H5A | 0.1051 | 0.6933 | 0.1711 | 0.034* |
| H5B | 0.0396 | 0.5964 | 0.1571 | 0.034* |
| C6 | 0.1087 (2) | 0.5702 (4) | 0.2895 (3) | 0.0276 (8) |
| H6A | 0.0757 | 0.5270 | 0.3161 | 0.033* |
| H6B | 0.1333 | 0.4885 | 0.2721 | 0.033* |
| C7 | 0.16265 (18) | 0.3824 (4) | 0.5421 (2) | 0.0232 (7) |
| H7 | 0.1946 | 0.3502 | 0.6033 | 0.028* |
| C8 | 0.1404 (2) | 0.2437 (4) | 0.4836 (3) | 0.0293 (8) |
| H8A | 0.1093 | 0.2709 | 0.4217 | 0.035* |
| H8B | 0.1794 | 0.1954 | 0.4735 | 0.035* |
| C9 | 0.1064 (2) | 0.1361 (4) | 0.5322 (3) | 0.0338 (9) |
| H9A | 0.0899 | 0.0502 | 0.4909 | 0.041* |
| H9B | 0.1392 | 0.1000 | 0.5905 | 0.041* |
| C10 | 0.04875 (19) | 0.2078 (4) | 0.5554 (3) | 0.0289 (8) |
| H10A | 0.0300 | 0.1371 | 0.5903 | 0.035* |
| H10B | 0.0135 | 0.2334 | 0.4967 | 0.035* |
| C11 | 0.0710 (2) | 0.3462 (4) | 0.6139 (3) | 0.0307 (9) |
| H11A | 0.1028 | 0.3193 | 0.6754 | 0.037* |
| H11B | 0.0322 | 0.3939 | 0.6248 | 0.037* |
| C12 | 0.10404 (19) | 0.4543 (4) | 0.5642 (3) | 0.0265 (8) |
| H12A | 0.0711 | 0.4879 | 0.5053 | 0.032* |
| H12B | 0.1198 | 0.5415 | 0.6044 | 0.032* |
| C13 | 0.28327 (18) | 0.6755 (4) | 0.5863 (2) | 0.0229 (7) |
| H13 | 0.3158 | 0.6080 | 0.6299 | 0.028* |
| C14 | 0.2482 (2) | 0.7634 (4) | 0.6445 (3) | 0.0302 (8) |
| H14A | 0.2135 | 0.8265 | 0.6024 | 0.036* |
| H14B | 0.2263 | 0.6943 | 0.6764 | 0.036* |
| C15 | 0.2972 (2) | 0.8594 (5) | 0.7173 (3) | 0.0399 (10) |
| H15A | 0.2729 | 0.9192 | 0.7509 | 0.048* |
| H15B | 0.3290 | 0.7957 | 0.7637 | 0.048* |
| C16 | 0.3352 (2) | 0.9610 (5) | 0.6714 (3) | 0.0399 (10) |
| H16A | 0.3039 | 1.0314 | 0.6299 | 0.048* |
| H16B | 0.3682 | 1.0182 | 0.7203 | 0.048* |
| C17 | 0.3701 (2) | 0.8748 (5) | 0.6152 (3) | 0.0350 (9) |
| H17A | 0.4047 | 0.8121 | 0.6579 | 0.042* |
| H17B | 0.3923 | 0.9440 | 0.5839 | 0.042* |
| C18 | 0.3220 (2) | 0.7777 (5) | 0.5415 (3) | 0.0333 (9) |
| H18A | 0.3472 | 0.7180 | 0.5092 | 0.040* |
| H18B | 0.2906 | 0.8407 | 0.4944 | 0.040* |
| C19 | 0.3064 (2) | 0.3375 (5) | 0.4512 (4) | 0.0428 (11) |
| C20 | 0.3465 (4) | 0.2732 (7) | 0.3902 (6) | 0.086 (2) |
| H20 | 0.3254 | 0.3114 | 0.3254 | 0.103* |
| C21 | 0.3511 (4) | 0.1324 (10) | 0.3833 (6) | 0.103 (3) |
| H21 | 0.3661 | 0.0957 | 0.4493 | 0.123* |
| C22 | 0.3980 (3) | 0.0619 (6) | 0.3377 (4) | 0.0589 (15) |
| C23 | 0.4391 (3) | -0.0514 (6) | 0.3837 (4) | 0.0600 (15) |
| H23 | 0.4393 | -0.0795 | 0.4445 | 0.072* |
| C24 | 0.4791 (3) | -0.1224 (6) | 0.3434 (3) | 0.0489 (12) |
| H24 | 0.5066 | -0.2006 | 0.3757 | 0.059* |

supplementary materials

| | | | | |
|-----|------------|-------------|------------|-------------|
| C25 | 0.4800 (2) | -0.0820 (5) | 0.2563 (3) | 0.0362 (10) |
| H25 | 0.5080 | -0.1328 | 0.2282 | 0.043* |
| C26 | 0.4408 (2) | 0.0312 (5) | 0.2089 (3) | 0.0345 (9) |
| H26 | 0.4420 | 0.0589 | 0.1486 | 0.041* |
| C27 | 0.3996 (2) | 0.1048 (5) | 0.2490 (3) | 0.0436 (11) |
| H27 | 0.3727 | 0.1837 | 0.2167 | 0.052* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|---------------|--------------|---------------|
| Sn1 | 0.02214 (13) | 0.02028 (12) | 0.02122 (12) | 0.00165 (10) | 0.00982 (9) | 0.00100 (10) |
| Br1 | 0.0356 (2) | 0.0413 (2) | 0.0301 (2) | -0.01657 (18) | 0.01398 (17) | -0.01001 (18) |
| Br2 | 0.0250 (2) | 0.0332 (2) | 0.0360 (2) | -0.00672 (16) | 0.01009 (16) | -0.00529 (17) |
| O1 | 0.0474 (18) | 0.0441 (18) | 0.0341 (16) | 0.0140 (15) | 0.0263 (14) | 0.0022 (14) |
| O2 | 0.0359 (17) | 0.0354 (17) | 0.062 (2) | 0.0099 (14) | 0.0122 (15) | 0.0110 (16) |
| C1 | 0.0203 (17) | 0.0223 (18) | 0.0237 (18) | 0.0007 (14) | 0.0074 (14) | 0.0011 (14) |
| C2 | 0.028 (2) | 0.0254 (19) | 0.0253 (19) | 0.0027 (16) | 0.0082 (15) | -0.0006 (15) |
| C3 | 0.031 (2) | 0.0236 (19) | 0.028 (2) | 0.0009 (16) | 0.0076 (16) | -0.0007 (16) |
| C4 | 0.0256 (19) | 0.032 (2) | 0.0227 (18) | -0.0020 (16) | 0.0040 (15) | 0.0050 (16) |
| C5 | 0.032 (2) | 0.029 (2) | 0.0205 (18) | -0.0075 (16) | 0.0043 (15) | -0.0031 (15) |
| C6 | 0.035 (2) | 0.0218 (19) | 0.0246 (19) | -0.0027 (16) | 0.0071 (16) | -0.0005 (15) |
| C7 | 0.0257 (19) | 0.0220 (18) | 0.0228 (18) | -0.0010 (15) | 0.0089 (15) | 0.0011 (14) |
| C8 | 0.034 (2) | 0.0249 (19) | 0.034 (2) | -0.0017 (16) | 0.0180 (17) | -0.0064 (16) |
| C9 | 0.042 (2) | 0.0209 (19) | 0.045 (2) | -0.0004 (17) | 0.023 (2) | -0.0037 (17) |
| C10 | 0.032 (2) | 0.0251 (19) | 0.033 (2) | -0.0035 (16) | 0.0154 (17) | -0.0015 (16) |
| C11 | 0.038 (2) | 0.028 (2) | 0.034 (2) | -0.0040 (17) | 0.0220 (18) | -0.0049 (17) |
| C12 | 0.031 (2) | 0.0194 (18) | 0.035 (2) | -0.0029 (16) | 0.0189 (17) | -0.0048 (16) |
| C13 | 0.0227 (18) | 0.0240 (18) | 0.0206 (17) | 0.0039 (15) | 0.0047 (14) | 0.0033 (14) |
| C14 | 0.033 (2) | 0.032 (2) | 0.029 (2) | -0.0006 (17) | 0.0143 (17) | -0.0025 (17) |
| C15 | 0.049 (3) | 0.043 (3) | 0.032 (2) | -0.010 (2) | 0.019 (2) | -0.013 (2) |
| C16 | 0.047 (3) | 0.030 (2) | 0.042 (2) | -0.010 (2) | 0.012 (2) | -0.0065 (19) |
| C17 | 0.037 (2) | 0.036 (2) | 0.032 (2) | -0.0117 (19) | 0.0109 (18) | 0.0017 (18) |
| C18 | 0.035 (2) | 0.039 (2) | 0.029 (2) | -0.0110 (18) | 0.0153 (17) | -0.0035 (18) |
| C19 | 0.043 (3) | 0.036 (2) | 0.058 (3) | 0.008 (2) | 0.028 (2) | -0.002 (2) |
| C20 | 0.089 (5) | 0.067 (4) | 0.129 (6) | 0.024 (4) | 0.073 (5) | -0.014 (4) |
| C21 | 0.088 (5) | 0.115 (6) | 0.129 (7) | -0.017 (5) | 0.069 (5) | -0.069 (6) |
| C22 | 0.073 (4) | 0.064 (4) | 0.059 (3) | -0.002 (3) | 0.048 (3) | -0.026 (3) |
| C23 | 0.096 (5) | 0.057 (3) | 0.039 (3) | -0.001 (3) | 0.039 (3) | -0.004 (3) |
| C24 | 0.058 (3) | 0.049 (3) | 0.036 (3) | 0.005 (2) | 0.008 (2) | -0.004 (2) |
| C25 | 0.028 (2) | 0.043 (2) | 0.041 (2) | -0.0025 (18) | 0.0155 (18) | -0.017 (2) |
| C26 | 0.045 (2) | 0.035 (2) | 0.030 (2) | -0.0115 (19) | 0.0210 (19) | -0.0097 (18) |
| C27 | 0.048 (3) | 0.033 (2) | 0.050 (3) | 0.006 (2) | 0.016 (2) | -0.012 (2) |

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

| | | | |
|---------|-----------|----------|--------|
| Sn1—O1 | 2.072 (3) | C11—H11A | 0.9900 |
| Sn1—C13 | 2.141 (4) | C11—H11B | 0.9900 |
| Sn1—C7 | 2.157 (3) | C12—H12A | 0.9900 |
| Sn1—C1 | 2.158 (3) | C12—H12B | 0.9900 |

| | | | |
|------------|-------------|---------------|------------|
| Br1—C20 | 2.054 (8) | C13—C18 | 1.530 (5) |
| Br2—C21 | 1.990 (7) | C13—C14 | 1.539 (5) |
| O1—C19 | 1.271 (5) | C13—H13 | 1.0000 |
| O2—C19 | 1.201 (6) | C14—C15 | 1.526 (6) |
| C1—C6 | 1.528 (5) | C14—H14A | 0.9900 |
| C1—C2 | 1.525 (5) | C14—H14B | 0.9900 |
| C1—H1 | 1.0000 | C15—C16 | 1.526 (6) |
| C2—C3 | 1.525 (5) | C15—H15A | 0.9900 |
| C2—H2A | 0.9900 | C15—H15B | 0.9900 |
| C2—H2B | 0.9900 | C16—C17 | 1.507 (6) |
| C3—C4 | 1.520 (5) | C16—H16A | 0.9900 |
| C3—H3A | 0.9900 | C16—H16B | 0.9900 |
| C3—H3B | 0.9900 | C17—C18 | 1.530 (6) |
| C4—C5 | 1.519 (5) | C17—H17A | 0.9900 |
| C4—H4A | 0.9900 | C17—H17B | 0.9900 |
| C4—H4B | 0.9900 | C18—H18A | 0.9900 |
| C5—C6 | 1.536 (5) | C18—H18B | 0.9900 |
| C5—H5A | 0.9900 | C19—C20 | 1.548 (7) |
| C5—H5B | 0.9900 | C20—C21 | 1.290 (10) |
| C6—H6A | 0.9900 | C20—H20 | 1.0000 |
| C6—H6B | 0.9900 | C21—C22 | 1.517 (7) |
| C7—C12 | 1.531 (5) | C21—H21 | 1.0000 |
| C7—C8 | 1.525 (5) | C22—C23 | 1.387 (8) |
| C7—H7 | 1.0000 | C22—C27 | 1.402 (7) |
| C8—C9 | 1.531 (5) | C23—C24 | 1.351 (7) |
| C8—H8A | 0.9900 | C23—H23 | 0.9500 |
| C8—H8B | 0.9900 | C24—C25 | 1.369 (6) |
| C9—C10 | 1.521 (5) | C24—H24 | 0.9500 |
| C9—H9A | 0.9900 | C25—C26 | 1.374 (6) |
| C9—H9B | 0.9900 | C25—H25 | 0.9500 |
| C10—C11 | 1.523 (5) | C26—C27 | 1.381 (6) |
| C10—H10A | 0.9900 | C26—H26 | 0.9500 |
| C10—H10B | 0.9900 | C27—H27 | 0.9500 |
| C11—C12 | 1.531 (5) | | |
| O1—Sn1—C13 | 107.13 (13) | C7—C12—H12A | 109.4 |
| O1—Sn1—C7 | 109.48 (13) | C11—C12—H12A | 109.4 |
| C13—Sn1—C7 | 114.25 (13) | C7—C12—H12B | 109.4 |
| O1—Sn1—C1 | 91.76 (12) | C11—C12—H12B | 109.4 |
| C13—Sn1—C1 | 112.88 (13) | H12A—C12—H12B | 108.0 |
| C7—Sn1—C1 | 118.36 (14) | C18—C13—C14 | 111.1 (3) |
| C19—O1—Sn1 | 115.9 (3) | C18—C13—Sn1 | 111.7 (2) |
| C6—C1—C2 | 111.1 (3) | C14—C13—Sn1 | 110.7 (2) |
| C6—C1—Sn1 | 112.5 (2) | C18—C13—H13 | 107.7 |
| C2—C1—Sn1 | 113.5 (2) | C14—C13—H13 | 107.7 |
| C6—C1—H1 | 106.4 | Sn1—C13—H13 | 107.7 |
| C2—C1—H1 | 106.4 | C15—C14—C13 | 111.2 (3) |
| Sn1—C1—H1 | 106.4 | C15—C14—H14A | 109.4 |
| C3—C2—C1 | 111.4 (3) | C13—C14—H14A | 109.4 |
| C3—C2—H2A | 109.3 | C15—C14—H14B | 109.4 |

supplementary materials

| | | | |
|--------------|-----------|---------------|-----------|
| C1—C2—H2A | 109.3 | C13—C14—H14B | 109.4 |
| C3—C2—H2B | 109.3 | H14A—C14—H14B | 108.0 |
| C1—C2—H2B | 109.3 | C16—C15—C14 | 111.0 (3) |
| H2A—C2—H2B | 108.0 | C16—C15—H15A | 109.4 |
| C4—C3—C2 | 111.7 (3) | C14—C15—H15A | 109.4 |
| C4—C3—H3A | 109.3 | C16—C15—H15B | 109.4 |
| C2—C3—H3A | 109.3 | C14—C15—H15B | 109.4 |
| C4—C3—H3B | 109.3 | H15A—C15—H15B | 108.0 |
| C2—C3—H3B | 109.3 | C17—C16—C15 | 111.2 (4) |
| H3A—C3—H3B | 107.9 | C17—C16—H16A | 109.4 |
| C3—C4—C5 | 111.5 (3) | C15—C16—H16A | 109.4 |
| C3—C4—H4A | 109.3 | C17—C16—H16B | 109.4 |
| C5—C4—H4A | 109.3 | C15—C16—H16B | 109.4 |
| C3—C4—H4B | 109.3 | H16A—C16—H16B | 108.0 |
| C5—C4—H4B | 109.3 | C16—C17—C18 | 111.9 (4) |
| H4A—C4—H4B | 108.0 | C16—C17—H17A | 109.2 |
| C4—C5—C6 | 111.3 (3) | C18—C17—H17A | 109.2 |
| C4—C5—H5A | 109.4 | C16—C17—H17B | 109.2 |
| C6—C5—H5A | 109.4 | C18—C17—H17B | 109.2 |
| C4—C5—H5B | 109.4 | H17A—C17—H17B | 107.9 |
| C6—C5—H5B | 109.4 | C17—C18—C13 | 111.0 (3) |
| H5A—C5—H5B | 108.0 | C17—C18—H18A | 109.4 |
| C1—C6—C5 | 111.1 (3) | C13—C18—H18A | 109.4 |
| C1—C6—H6A | 109.4 | C17—C18—H18B | 109.4 |
| C5—C6—H6A | 109.4 | C13—C18—H18B | 109.4 |
| C1—C6—H6B | 109.4 | H18A—C18—H18B | 108.0 |
| C5—C6—H6B | 109.4 | O2—C19—O1 | 125.8 (4) |
| H6A—C6—H6B | 108.0 | O2—C19—C20 | 122.6 (5) |
| C12—C7—C8 | 110.6 (3) | O1—C19—C20 | 111.6 (5) |
| C12—C7—Sn1 | 110.2 (2) | C21—C20—C19 | 119.5 (6) |
| C8—C7—Sn1 | 115.3 (2) | C21—C20—Br1 | 112.1 (6) |
| C12—C7—H7 | 106.7 | C19—C20—Br1 | 104.4 (4) |
| C8—C7—H7 | 106.7 | C21—C20—H20 | 106.7 |
| Sn1—C7—H7 | 106.7 | C19—C20—H20 | 106.7 |
| C9—C8—C7 | 111.0 (3) | Br1—C20—H20 | 106.7 |
| C9—C8—H8A | 109.4 | C20—C21—C22 | 122.2 (7) |
| C7—C8—H8A | 109.4 | C20—C21—Br2 | 105.6 (6) |
| C9—C8—H8B | 109.4 | C22—C21—Br2 | 112.6 (4) |
| C7—C8—H8B | 109.4 | C20—C21—H21 | 105.0 |
| H8A—C8—H8B | 108.0 | C22—C21—H21 | 105.0 |
| C10—C9—C8 | 111.8 (3) | Br2—C21—H21 | 105.0 |
| C10—C9—H9A | 109.3 | C23—C22—C27 | 118.8 (4) |
| C8—C9—H9A | 109.3 | C23—C22—C21 | 119.1 (6) |
| C10—C9—H9B | 109.3 | C27—C22—C21 | 122.0 (6) |
| C8—C9—H9B | 109.3 | C24—C23—C22 | 121.1 (5) |
| H9A—C9—H9B | 107.9 | C24—C23—H23 | 119.5 |
| C9—C10—C11 | 111.1 (3) | C22—C23—H23 | 119.5 |
| C9—C10—H10A | 109.4 | C23—C24—C25 | 120.1 (5) |
| C11—C10—H10A | 109.4 | C23—C24—H24 | 119.9 |

| | | | |
|----------------|------------|-----------------|------------|
| C9—C10—H10B | 109.4 | C25—C24—H24 | 119.9 |
| C11—C10—H10B | 109.4 | C24—C25—C26 | 120.6 (4) |
| H10A—C10—H10B | 108.0 | C24—C25—H25 | 119.7 |
| C10—C11—C12 | 110.7 (3) | C26—C25—H25 | 119.7 |
| C10—C11—H11A | 109.5 | C25—C26—C27 | 120.0 (4) |
| C12—C11—H11A | 109.5 | C25—C26—H26 | 120.0 |
| C10—C11—H11B | 109.5 | C27—C26—H26 | 120.0 |
| C12—C11—H11B | 109.5 | C26—C27—C22 | 119.4 (5) |
| H11A—C11—H11B | 108.1 | C26—C27—H27 | 120.3 |
| C7—C12—C11 | 111.1 (3) | C22—C27—H27 | 120.3 |
| C13—Sn1—O1—C19 | 69.2 (3) | O1—Sn1—C13—C14 | 178.1 (2) |
| C7—Sn1—O1—C19 | -55.2 (3) | C7—Sn1—C13—C14 | -60.5 (3) |
| C1—Sn1—O1—C19 | -176.2 (3) | C1—Sn1—C13—C14 | 78.6 (3) |
| O1—Sn1—C1—C6 | 69.1 (3) | C18—C13—C14—C15 | -54.9 (4) |
| C13—Sn1—C1—C6 | 178.5 (2) | Sn1—C13—C14—C15 | -179.7 (3) |
| C7—Sn1—C1—C6 | -44.2 (3) | C13—C14—C15—C16 | 55.5 (5) |
| O1—Sn1—C1—C2 | -163.7 (3) | C14—C15—C16—C17 | -56.1 (5) |
| C13—Sn1—C1—C2 | -54.2 (3) | C15—C16—C17—C18 | 56.1 (5) |
| C7—Sn1—C1—C2 | 83.0 (3) | C16—C17—C18—C13 | -55.3 (5) |
| C6—C1—C2—C3 | -55.1 (4) | C14—C13—C18—C17 | 54.2 (4) |
| Sn1—C1—C2—C3 | 176.9 (2) | Sn1—C13—C18—C17 | 178.4 (3) |
| C1—C2—C3—C4 | 54.8 (4) | Sn1—O1—C19—O2 | 3.9 (7) |
| C2—C3—C4—C5 | -54.7 (4) | Sn1—O1—C19—C20 | -175.7 (4) |
| C3—C4—C5—C6 | 54.9 (4) | O2—C19—C20—C21 | 49.4 (11) |
| C2—C1—C6—C5 | 55.4 (4) | O1—C19—C20—C21 | -131.0 (8) |
| Sn1—C1—C6—C5 | -176.1 (2) | O2—C19—C20—Br1 | -76.9 (6) |
| C4—C5—C6—C1 | -55.3 (4) | O1—C19—C20—Br1 | 102.7 (5) |
| O1—Sn1—C7—C12 | -157.5 (2) | C19—C20—C21—C22 | -170.2 (6) |
| C13—Sn1—C7—C12 | 82.4 (3) | Br1—C20—C21—C22 | -47.6 (11) |
| C1—Sn1—C7—C12 | -54.3 (3) | C19—C20—C21—Br2 | 59.5 (9) |
| O1—Sn1—C7—C8 | -31.4 (3) | Br1—C20—C21—Br2 | -177.9 (3) |
| C13—Sn1—C7—C8 | -151.5 (3) | C20—C21—C22—C23 | 131.4 (9) |
| C1—Sn1—C7—C8 | 71.8 (3) | Br2—C21—C22—C23 | -101.3 (7) |
| C12—C7—C8—C9 | -55.5 (4) | C20—C21—C22—C27 | -50.6 (11) |
| Sn1—C7—C8—C9 | 178.6 (3) | Br2—C21—C22—C27 | 76.7 (7) |
| C7—C8—C9—C10 | 55.3 (5) | C27—C22—C23—C24 | -1.7 (9) |
| C8—C9—C10—C11 | -55.4 (5) | C21—C22—C23—C24 | 176.4 (6) |
| C9—C10—C11—C12 | 55.8 (5) | C22—C23—C24—C25 | 0.7 (9) |
| C8—C7—C12—C11 | 56.6 (4) | C23—C24—C25—C26 | 0.4 (8) |
| Sn1—C7—C12—C11 | -174.7 (3) | C24—C25—C26—C27 | -0.5 (7) |
| C10—C11—C12—C7 | -56.7 (4) | C25—C26—C27—C22 | -0.5 (7) |
| O1—Sn1—C13—C18 | 53.7 (3) | C23—C22—C27—C26 | 1.5 (8) |
| C7—Sn1—C13—C18 | 175.1 (3) | C21—C22—C27—C26 | -176.5 (5) |
| C1—Sn1—C13—C18 | -45.8 (3) | | |

Fig. 1

