

Dichloridoctakis(2-chlorobenzyl)di- μ_2 -hydroxido-di- μ_3 -oxido-tetratin(IV)

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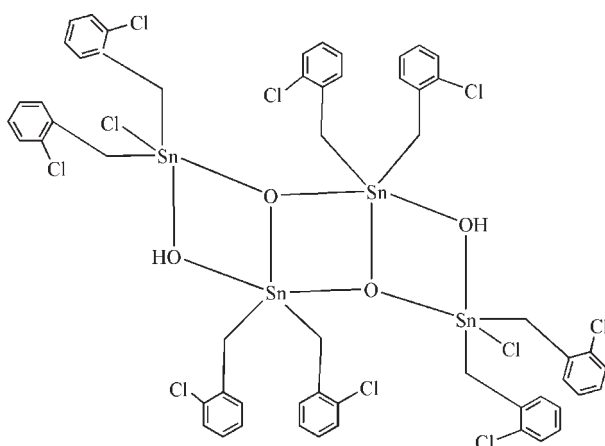
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; disorder in main residue; R factor = 0.029; wR factor = 0.074; data-to-parameter ratio = 15.1.

The title tetranuclear Sn^{IV} compound, $[\text{Sn}_4(\text{C}_7\text{H}_6\text{Cl})_8\text{Cl}_2\text{O}_2(\text{OH})_2]$, has site symmetry $\bar{1}$. Two O^{2-} and two OH^- anions bridge four Sn^{IV} cations to form the tetranuclear compound. The two independent Sn^{IV} cations assume SnO_3C_2 and $\text{SnO}_2\text{C}_2\text{Cl}$ distorted trigonal-bipyramidal coordination geometries. Intramolecular $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonding is present in the structure. One Cl atom of a chlorobenzyl ligand is disordered over two sites with an occupancy ratio of 0.693 (2):0.307 (2).

Related literature

For a related structure, see: Li *et al.* (2006). For the corresponding bond distances in an organotin compound, see: Lo & Ng (2009).



Experimental

Crystal data

$[\text{Sn}_4(\text{C}_7\text{H}_6\text{Cl})_8\text{Cl}_2\text{O}_2(\text{OH})_2]$
 $M_r = 1616.22$
 Triclinic, $P\bar{1}$
 $a = 10.986$ (2) Å
 $b = 11.227$ (2) Å
 $c = 13.573$ (3) Å
 $\alpha = 74.656$ (2)°
 $\beta = 67.942$ (2)°

$\gamma = 75.753$ (2)°
 $V = 1475.9$ (6) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 2.17$ mm⁻¹
 $T = 298$ K
 $0.44 \times 0.37 \times 0.33$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.449$, $T_{\max} = 0.535$
 7669 measured reflections
 5112 independent reflections
 3865 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.015$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.074$
 $S = 1.04$
 5112 reflections
 338 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 1.27$ e Å⁻³
 $\Delta\rho_{\min} = -0.57$ e Å⁻³

Table 1

Selected bond lengths (Å).

| | | | |
|---------------------|-----------|---------|-------------|
| Sn1—O1 | 2.148 (3) | Sn2—O1 | 2.276 (3) |
| Sn1—O2 | 2.050 (3) | Sn2—O2 | 2.025 (3) |
| Sn1—O2 ⁱ | 2.146 (3) | Sn2—C15 | 2.147 (5) |
| Sn1—C1 | 2.126 (5) | Sn2—C22 | 2.149 (5) |
| Sn1—C8 | 2.146 (5) | Sn2—C11 | 2.4376 (13) |

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

Table 2

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|-------------------------|--------------|--------------------|-------------|----------------------|
| O1—H1 ⁱ ⋯Cl2 | 0.86 | 2.80 | 3.386 (4) | 127 |

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; 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: XU2652).

References

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supplementary materials

Acta Cryst. (2009). E65, m1494 [doi:10.1107/S1600536809045176]

Dichloridoctakis(2-chlorobenzyl)di- μ_2 -hydroxido-di- μ_3 -oxido-tetratin(IV)

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Comment

The title compound, (I), was obtained as an adventitious product of the partial hydrolysis of di(2-chlorobenzyl)dichloridotin(IV) during the attempted preparation of adducts of this tin precursor complex with 5-chlorosalicylaldehyde benzoyldrazone in benzene and ethanol. It crystallizes from dichloromethane and ethanol. From Fig. 1, it can be seen that complex (I) contains two independent penta-coordinated Sn atoms. It is a centrosymmetric complex, where one half of the molecule comprises the crystallographic asymmetric unit and the other half is generated by an inversion centre. Each of the two independent Sn atoms is five-coordinate, adopting approximate trigonal bipyramidal coordination (Table 1). These are similar to those in the related organotin compound (Li *et al.*, 2006). The molecular conformation is stabilized by O1—H1...Cl2 hydrogen bond (Table 2). The Sn—C distances lie in the rather narrow range 2.126 (5)–2.149 (5) Å, which are closed to the corresponding distances reported in the organotin compound (Lo & Ng, 2009).

Experimental

Di(2-chlorobenzyl)dichloridotin(IV) (2 mmol) and 5-chlorosalicylaldehyde benzoyldrazone(2 mmol) was added to a solution of sodium methoxide (3 mmol) in benzene (15 ml) and ethanol (15 ml, 95%). The mixture was then heated under reflux with stirring for 5 h and the solvent was removed by evaporation in vacuo. The crude adduct was recrystallized from dichloromethane/ethanol and colourless crystals suitable for X-ray diffraction were obtained.

Refinement

The H atoms were positioned geometrically, with methylene C—H distances of 0.97 Å, aromatic C—H distances of 0.93 Å, O—H distances of 0.862 Å and refined as riding on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}, \text{O})$. The Cl2 atom is disordered, the C2-phenyl part was refined as a rigid hexagon and the temperature factors of the carbon atoms were restrained to be nearly isotropic. The highest peak in the difference map is 1.21 Å apart from Cl1 atom.

Figures

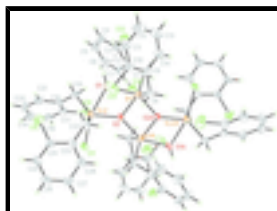


Fig. 1. The molecular structure of the compound showing 50% probability displacement ellipsoids [symmetry code: (A) = 1-x, 1-y, 1-z].

Dichloridoctakis(2-chlorobenzyl)di- μ_2 -hydroxido-di- μ_3 -oxido-tetratin(IV)

Crystal data

| | |
|--|---|
| $[\text{Sn}_4(\text{C}_7\text{H}_6\text{Cl})_8\text{Cl}_2\text{O}_2(\text{OH})_2]$ | $Z = 1$ |
| $M_r = 1616.22$ | $F(000) = 788$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.818 \text{ Mg m}^{-3}$ |
| Hall symbol: $-P\ 1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| $a = 10.986 (2) \text{ \AA}$ | Cell parameters from 4036 reflections |
| $b = 11.227 (2) \text{ \AA}$ | $\theta = 2.6\text{--}27.4^\circ$ |
| $c = 13.573 (3) \text{ \AA}$ | $\mu = 2.17 \text{ mm}^{-1}$ |
| $\alpha = 74.656 (2)^\circ$ | $T = 298 \text{ K}$ |
| $\beta = 67.942 (2)^\circ$ | Block, colourless |
| $\gamma = 75.753 (2)^\circ$ | $0.44 \times 0.37 \times 0.33 \text{ mm}$ |
| $V = 1475.9 (6) \text{ \AA}^3$ | |

Data collection

| | |
|---|--|
| Bruker SMART CCD area-detector diffractometer | 5112 independent reflections |
| Radiation source: fine-focus sealed tube graphite | 3865 reflections with $I > 2\sigma(I)$ |
| φ and ω scans | $R_{\text{int}} = 0.015$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 1.7^\circ$ |
| $T_{\text{min}} = 0.449$, $T_{\text{max}} = 0.535$ | $h = -13 \rightarrow 13$ |
| 7669 measured reflections | $k = -13 \rightarrow 13$ |
| | $l = -16 \rightarrow 10$ |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.029$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.074$ | H-atom parameters constrained |
| $S = 1.04$ | $w = 1/[\sigma^2(F_o^2) + (0.0262P)^2 + 2.2448P]$ |
| 5112 reflections | where $P = (F_o^2 + 2F_c^2)/3$ |
| 338 parameters | $(\Delta/\sigma)_{\text{max}} = 0.001$ |
| 0 restraints | $\Delta\rho_{\text{max}} = 1.27 \text{ e \AA}^{-3}$ |
| | $\Delta\rho_{\text{min}} = -0.57 \text{ e \AA}^{-3}$ |

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|-----|-------------|-------------|-------------|----------------------------------|-----------|
| Sn1 | 0.59257 (3) | 0.37338 (3) | 0.44839 (2) | 0.03438 (10) | |

| | | | | | |
|------|--------------|--------------|---------------|--------------|-----------|
| Sn2 | 0.49384 (3) | 0.58881 (3) | 0.25330 (2) | 0.03713 (10) | |
| C11 | 0.35586 (14) | 0.79133 (11) | 0.28147 (11) | 0.0516 (3) | |
| C12 | 0.6318 (2) | 0.0780 (2) | 0.34868 (19) | 0.0704 (6) | 0.693 (2) |
| C12' | 0.2326 (5) | 0.3325 (5) | 0.5648 (4) | 0.0704 (6) | 0.307 (2) |
| C13 | 0.96390 (18) | 0.40745 (16) | 0.17259 (15) | 0.0897 (6) | |
| C14 | 0.09931 (19) | 0.5877 (2) | 0.36984 (14) | 0.0927 (6) | |
| C15 | 0.6057 (2) | 0.72167 (16) | -0.03870 (14) | 0.0908 (6) | |
| O1 | 0.6121 (3) | 0.3933 (3) | 0.2815 (2) | 0.0444 (8) | |
| H1 | 0.6408 | 0.3297 | 0.2503 | 0.053* | |
| O2 | 0.4776 (3) | 0.5414 (3) | 0.4119 (2) | 0.0365 (7) | |
| C1 | 0.4860 (7) | 0.2203 (6) | 0.5202 (5) | 0.077 (2) | |
| H1A | 0.5486 | 0.1446 | 0.5314 | 0.092* | |
| H1B | 0.4238 | 0.2336 | 0.5908 | 0.092* | |
| C2 | 0.4103 (7) | 0.2003 (5) | 0.4555 (5) | 0.0597 (16) | |
| C3 | 0.4702 (6) | 0.1302 (5) | 0.3739 (5) | 0.0646 (17) | |
| H3A | 0.5605 | 0.0982 | 0.3588 | 0.077* | 0.307 (2) |
| C4 | 0.4013 (7) | 0.1078 (6) | 0.3160 (5) | 0.0697 (18) | |
| H4 | 0.4440 | 0.0592 | 0.2629 | 0.084* | |
| C5 | 0.2691 (8) | 0.1581 (7) | 0.3376 (6) | 0.078 (2) | |
| H5 | 0.2210 | 0.1431 | 0.2998 | 0.093* | |
| C6 | 0.2087 (7) | 0.2301 (6) | 0.4146 (6) | 0.0775 (19) | |
| H6 | 0.1197 | 0.2663 | 0.4277 | 0.093* | |
| C7 | 0.2776 (8) | 0.2497 (6) | 0.4731 (5) | 0.0724 (18) | |
| H7A | 0.2335 | 0.2980 | 0.5263 | 0.087* | 0.693 (2) |
| C8 | 0.8018 (5) | 0.3527 (5) | 0.4200 (4) | 0.0541 (14) | |
| H8A | 0.8337 | 0.4296 | 0.3766 | 0.065* | |
| H8B | 0.8166 | 0.3377 | 0.4887 | 0.065* | |
| C9 | 0.8788 (5) | 0.2460 (5) | 0.3625 (4) | 0.0469 (12) | |
| C10 | 0.9489 (5) | 0.2595 (5) | 0.2531 (4) | 0.0510 (13) | |
| C11 | 1.0141 (5) | 0.1589 (6) | 0.2019 (5) | 0.0630 (16) | |
| H11 | 1.0598 | 0.1719 | 0.1278 | 0.076* | |
| C12 | 1.0104 (6) | 0.0399 (6) | 0.2620 (6) | 0.080 (2) | |
| H12 | 1.0524 | -0.0287 | 0.2285 | 0.096* | |
| C13 | 0.9448 (7) | 0.0222 (6) | 0.3713 (7) | 0.086 (2) | |
| H13 | 0.9450 | -0.0587 | 0.4121 | 0.103* | |
| C14 | 0.8791 (6) | 0.1218 (6) | 0.4213 (5) | 0.0666 (16) | |
| H14 | 0.8337 | 0.1074 | 0.4955 | 0.080* | |
| C15 | 0.3720 (6) | 0.5022 (5) | 0.2102 (4) | 0.0541 (14) | |
| H15A | 0.4308 | 0.4523 | 0.1568 | 0.065* | |
| H15B | 0.3287 | 0.4446 | 0.2740 | 0.065* | |
| C16 | 0.2673 (6) | 0.5833 (5) | 0.1664 (4) | 0.0488 (13) | |
| C17 | 0.1427 (6) | 0.6287 (5) | 0.2294 (5) | 0.0596 (15) | |
| C18 | 0.0470 (7) | 0.7033 (6) | 0.1868 (6) | 0.0728 (18) | |
| H18 | -0.0357 | 0.7343 | 0.2323 | 0.087* | |
| C19 | 0.0748 (7) | 0.7312 (6) | 0.0775 (6) | 0.080 (2) | |
| H19 | 0.0110 | 0.7812 | 0.0480 | 0.096* | |
| C20 | 0.1997 (8) | 0.6846 (6) | 0.0096 (5) | 0.0760 (19) | |
| H20 | 0.2185 | 0.7022 | -0.0650 | 0.091* | |
| C21 | 0.2924 (6) | 0.6141 (5) | 0.0526 (5) | 0.0632 (16) | |

supplementary materials

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|------|------------|------------|-------------|-------------|
| H21 | 0.3754 | 0.5846 | 0.0065 | 0.076* |
| C22 | 0.6829 (5) | 0.6492 (5) | 0.1629 (4) | 0.0546 (14) |
| H22A | 0.7318 | 0.6346 | 0.2126 | 0.066* |
| H22B | 0.7322 | 0.5957 | 0.1103 | 0.066* |
| C23 | 0.6833 (5) | 0.7819 (4) | 0.1041 (4) | 0.0445 (12) |
| C24 | 0.6538 (5) | 0.8249 (5) | 0.0094 (4) | 0.0491 (13) |
| C25 | 0.6586 (6) | 0.9448 (5) | -0.0481 (4) | 0.0566 (14) |
| H25 | 0.6375 | 0.9697 | -0.1116 | 0.068* |
| C26 | 0.6952 (6) | 1.0277 (5) | -0.0102 (5) | 0.0672 (17) |
| H26 | 0.7000 | 1.1093 | -0.0487 | 0.081* |
| C27 | 0.7244 (7) | 0.9914 (6) | 0.0830 (5) | 0.0712 (18) |
| H27 | 0.7487 | 1.0480 | 0.1085 | 0.085* |
| C28 | 0.7178 (6) | 0.8692 (6) | 0.1404 (5) | 0.0666 (16) |
| H28 | 0.7370 | 0.8454 | 0.2047 | 0.080* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|------|-------------|--------------|--------------|---------------|---------------|---------------|
| Sn1 | 0.0413 (2) | 0.02862 (17) | 0.03475 (19) | -0.00165 (14) | -0.01569 (15) | -0.00788 (13) |
| Sn2 | 0.0458 (2) | 0.03431 (18) | 0.03224 (19) | -0.00562 (15) | -0.01628 (15) | -0.00401 (14) |
| Cl1 | 0.0610 (8) | 0.0372 (6) | 0.0546 (8) | 0.0030 (6) | -0.0240 (7) | -0.0085 (6) |
| Cl2 | 0.0727 (14) | 0.0590 (12) | 0.0858 (15) | -0.0032 (10) | -0.0315 (12) | -0.0237 (10) |
| Cl2' | 0.0727 (14) | 0.0590 (12) | 0.0858 (15) | -0.0032 (10) | -0.0315 (12) | -0.0237 (10) |
| Cl3 | 0.0743 (11) | 0.0692 (11) | 0.0932 (13) | -0.0020 (9) | -0.0141 (10) | 0.0080 (9) |
| Cl4 | 0.0917 (13) | 0.1304 (16) | 0.0571 (10) | -0.0280 (12) | -0.0216 (9) | -0.0155 (10) |
| Cl5 | 0.1487 (18) | 0.0662 (10) | 0.0763 (12) | -0.0408 (11) | -0.0494 (12) | -0.0049 (8) |
| O1 | 0.054 (2) | 0.0381 (18) | 0.0397 (19) | -0.0030 (16) | -0.0209 (16) | -0.0015 (14) |
| O2 | 0.0440 (19) | 0.0304 (16) | 0.0341 (17) | 0.0006 (14) | -0.0169 (15) | -0.0051 (13) |
| C1 | 0.137 (6) | 0.064 (4) | 0.056 (4) | -0.059 (4) | -0.052 (4) | 0.014 (3) |
| C2 | 0.097 (5) | 0.048 (3) | 0.048 (3) | -0.043 (3) | -0.034 (3) | 0.011 (3) |
| C3 | 0.081 (5) | 0.060 (4) | 0.067 (4) | -0.028 (3) | -0.041 (4) | 0.003 (3) |
| C4 | 0.099 (5) | 0.068 (4) | 0.063 (4) | -0.032 (4) | -0.038 (4) | -0.013 (3) |
| C5 | 0.093 (6) | 0.082 (5) | 0.084 (5) | -0.041 (4) | -0.051 (4) | -0.002 (4) |
| C6 | 0.074 (5) | 0.074 (4) | 0.090 (5) | -0.029 (4) | -0.031 (4) | -0.003 (4) |
| C7 | 0.101 (6) | 0.065 (4) | 0.061 (4) | -0.042 (4) | -0.027 (4) | 0.000 (3) |
| C8 | 0.047 (3) | 0.063 (4) | 0.064 (4) | 0.000 (3) | -0.022 (3) | -0.033 (3) |
| C9 | 0.035 (3) | 0.054 (3) | 0.055 (3) | -0.001 (2) | -0.019 (2) | -0.016 (3) |
| C10 | 0.039 (3) | 0.058 (3) | 0.058 (4) | -0.003 (3) | -0.020 (3) | -0.013 (3) |
| C11 | 0.045 (3) | 0.075 (4) | 0.068 (4) | 0.005 (3) | -0.015 (3) | -0.031 (3) |
| C12 | 0.062 (4) | 0.068 (4) | 0.108 (6) | 0.004 (3) | -0.016 (4) | -0.044 (4) |
| C13 | 0.069 (5) | 0.052 (4) | 0.112 (6) | -0.008 (3) | -0.016 (4) | 0.003 (4) |
| C14 | 0.051 (4) | 0.064 (4) | 0.069 (4) | 0.004 (3) | -0.014 (3) | -0.007 (3) |
| C15 | 0.065 (4) | 0.048 (3) | 0.060 (4) | -0.013 (3) | -0.029 (3) | -0.013 (3) |
| C16 | 0.061 (4) | 0.045 (3) | 0.055 (3) | -0.013 (3) | -0.030 (3) | -0.014 (2) |
| C17 | 0.063 (4) | 0.067 (4) | 0.057 (4) | -0.013 (3) | -0.026 (3) | -0.015 (3) |
| C18 | 0.064 (4) | 0.079 (4) | 0.085 (5) | -0.005 (3) | -0.038 (4) | -0.020 (4) |
| C19 | 0.082 (5) | 0.077 (5) | 0.095 (6) | -0.004 (4) | -0.057 (5) | -0.005 (4) |
| C20 | 0.106 (6) | 0.083 (5) | 0.058 (4) | -0.030 (4) | -0.045 (4) | -0.005 (3) |

| | | | | | | |
|-----|-----------|-----------|-----------|------------|------------|------------|
| C21 | 0.066 (4) | 0.063 (4) | 0.074 (4) | -0.011 (3) | -0.030 (3) | -0.025 (3) |
| C22 | 0.047 (3) | 0.046 (3) | 0.058 (3) | -0.004 (2) | -0.016 (3) | 0.005 (3) |
| C23 | 0.033 (3) | 0.041 (3) | 0.048 (3) | -0.006 (2) | -0.006 (2) | -0.002 (2) |
| C24 | 0.049 (3) | 0.044 (3) | 0.047 (3) | -0.008 (2) | -0.009 (3) | -0.006 (2) |
| C25 | 0.064 (4) | 0.046 (3) | 0.048 (3) | -0.005 (3) | -0.013 (3) | -0.002 (3) |
| C26 | 0.072 (4) | 0.039 (3) | 0.070 (4) | -0.002 (3) | -0.007 (3) | -0.007 (3) |
| C27 | 0.089 (5) | 0.065 (4) | 0.062 (4) | -0.033 (4) | -0.011 (4) | -0.016 (3) |
| C28 | 0.065 (4) | 0.076 (4) | 0.061 (4) | -0.020 (3) | -0.024 (3) | -0.005 (3) |

Geometric parameters (Å, °)

| | | | |
|---------------------|-------------|-----------|-----------|
| Sn1—O1 | 2.148 (3) | C9—C14 | 1.412 (7) |
| Sn1—O2 | 2.050 (3) | C10—C11 | 1.385 (8) |
| Sn1—O2 ⁱ | 2.146 (3) | C11—C12 | 1.370 (8) |
| Sn1—C1 | 2.126 (5) | C11—H11 | 0.9300 |
| Sn1—C8 | 2.146 (5) | C12—C13 | 1.368 (9) |
| Sn2—O1 | 2.276 (3) | C12—H12 | 0.9300 |
| Sn2—O2 | 2.025 (3) | C13—C14 | 1.367 (9) |
| Sn2—C15 | 2.147 (5) | C13—H13 | 0.9300 |
| Sn2—C22 | 2.149 (5) | C14—H14 | 0.9300 |
| Sn2—C11 | 2.4376 (13) | C15—C16 | 1.489 (7) |
| C12—C3 | 1.658 (7) | C15—H15A | 0.9700 |
| C12—H3A | 0.7301 | C15—H15B | 0.9700 |
| C12'—C7 | 1.606 (8) | C16—C17 | 1.368 (8) |
| C12'—H7A | 0.7242 | C16—C21 | 1.424 (7) |
| C13—C10 | 1.737 (6) | C17—C18 | 1.381 (8) |
| C14—C17 | 1.742 (6) | C18—C19 | 1.361 (9) |
| C15—C24 | 1.735 (5) | C18—H18 | 0.9300 |
| O1—H1 | 0.8590 | C19—C20 | 1.399 (9) |
| C1—C2 | 1.503 (7) | C19—H19 | 0.9300 |
| C1—H1A | 0.9700 | C20—C21 | 1.345 (8) |
| C1—H1B | 0.9700 | C20—H20 | 0.9300 |
| C2—C7 | 1.379 (9) | C21—H21 | 0.9300 |
| C2—C3 | 1.391 (8) | C22—C23 | 1.492 (6) |
| C3—C4 | 1.379 (7) | C22—H22A | 0.9700 |
| C3—H3A | 0.9301 | C22—H22B | 0.9700 |
| C4—C5 | 1.371 (9) | C23—C24 | 1.377 (7) |
| C4—H4 | 0.9300 | C23—C28 | 1.388 (7) |
| C5—C6 | 1.359 (9) | C24—C25 | 1.369 (7) |
| C5—H5 | 0.9300 | C25—C26 | 1.374 (8) |
| C6—C7 | 1.371 (8) | C25—H25 | 0.9300 |
| C6—H6 | 0.9300 | C26—C27 | 1.355 (8) |
| C7—H7A | 0.9300 | C26—H26 | 0.9300 |
| C8—C9 | 1.502 (7) | C27—C28 | 1.391 (8) |
| C8—H8A | 0.9700 | C27—H27 | 0.9300 |
| C8—H8B | 0.9700 | C28—H28 | 0.9300 |
| C9—C10 | 1.379 (7) | | |
| O2—Sn1—C1 | 114.2 (2) | C10—C9—C8 | 124.6 (5) |

supplementary materials

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| O2—Sn1—O2 ⁱ | 73.49 (12) | C14—C9—C8 | 119.6 (5) |
| C1—Sn1—O2 ⁱ | 97.25 (19) | C9—C10—C11 | 123.1 (5) |
| O2—Sn1—C8 | 123.37 (17) | C9—C10—C13 | 120.6 (4) |
| C1—Sn1—C8 | 122.4 (3) | C11—C10—C13 | 116.3 (5) |
| O2 ⁱ —Sn1—C8 | 97.54 (16) | C12—C11—C10 | 119.1 (6) |
| O2—Sn1—O1 | 74.51 (12) | C12—C11—H11 | 120.5 |
| C1—Sn1—O1 | 100.54 (17) | C10—C11—H11 | 120.5 |
| O2 ⁱ —Sn1—O1 | 147.55 (11) | C13—C12—C11 | 119.8 (6) |
| C8—Sn1—O1 | 95.50 (17) | C13—C12—H12 | 120.1 |
| O2—Sn2—C15 | 114.44 (17) | C11—C12—H12 | 120.1 |
| O2—Sn2—C22 | 108.14 (17) | C14—C13—C12 | 120.9 (6) |
| C15—Sn2—C22 | 131.7 (2) | C14—C13—H13 | 119.6 |
| O2—Sn2—O1 | 72.21 (11) | C12—C13—H13 | 119.6 |
| C15—Sn2—O1 | 85.91 (16) | C13—C14—C9 | 121.3 (6) |
| C22—Sn2—O1 | 86.30 (16) | C13—C14—H14 | 119.4 |
| O2—Sn2—C11 | 90.33 (9) | C9—C14—H14 | 119.4 |
| C15—Sn2—C11 | 102.16 (15) | C16—C15—Sn2 | 118.8 (3) |
| C22—Sn2—C11 | 99.22 (15) | C16—C15—H15A | 107.6 |
| O1—Sn2—C11 | 162.53 (9) | Sn2—C15—H15A | 107.6 |
| C3—C12—H3A | 3.0 | C16—C15—H15B | 107.6 |
| C7—C12 ⁱ —H7A | 15.7 | Sn2—C15—H15B | 107.6 |
| Sn1—O1—Sn2 | 100.13 (13) | H15A—C15—H15B | 107.0 |
| Sn1—O1—H1 | 120.9 | C17—C16—C21 | 115.9 (5) |
| Sn2—O1—H1 | 137.0 | C17—C16—C15 | 124.1 (5) |
| Sn2—O2—Sn1 | 112.76 (14) | C21—C16—C15 | 119.9 (5) |
| Sn2—O2—Sn1 ⁱ | 139.33 (14) | C16—C17—C18 | 123.0 (6) |
| Sn1—O2—Sn1 ⁱ | 106.51 (12) | C16—C17—C14 | 119.2 (4) |
| C2—C1—Sn1 | 114.9 (3) | C18—C17—C14 | 117.8 (5) |
| C2—C1—H1A | 108.5 | C19—C18—C17 | 119.4 (6) |
| Sn1—C1—H1A | 108.5 | C19—C18—H18 | 120.3 |
| C2—C1—H1B | 108.5 | C17—C18—H18 | 120.3 |
| Sn1—C1—H1B | 108.5 | C18—C19—C20 | 119.8 (6) |
| H1A—C1—H1B | 107.5 | C18—C19—H19 | 120.1 |
| C7—C2—C3 | 115.8 (5) | C20—C19—H19 | 120.1 |
| C7—C2—C1 | 122.3 (6) | C21—C20—C19 | 119.8 (6) |
| C3—C2—C1 | 121.9 (6) | C21—C20—H20 | 120.1 |
| C4—C3—C2 | 122.6 (6) | C19—C20—H20 | 120.1 |
| C4—C3—C12 | 121.9 (6) | C20—C21—C16 | 122.0 (6) |
| C2—C3—C12 | 115.4 (5) | C20—C21—H21 | 119.0 |
| C4—C3—H3A | 119.9 | C16—C21—H21 | 119.0 |
| C2—C3—H3A | 117.5 | C23—C22—Sn2 | 118.1 (3) |
| C12—C3—H3A | 2.4 | C23—C22—H22A | 107.8 |
| C5—C4—C3 | 119.1 (6) | Sn2—C22—H22A | 107.8 |
| C5—C4—H4 | 120.5 | C23—C22—H22B | 107.8 |
| C3—C4—H4 | 120.5 | Sn2—C22—H22B | 107.8 |
| C6—C5—C4 | 119.7 (6) | H22A—C22—H22B | 107.1 |
| C6—C5—H5 | 120.2 | C24—C23—C28 | 115.7 (5) |
| C4—C5—H5 | 120.2 | C24—C23—C22 | 122.7 (5) |

| | | | |
|--|--------------|-----------------|------------|
| C5—C6—C7 | 120.7 (7) | C28—C23—C22 | 121.5 (5) |
| C5—C6—H6 | 119.7 | C25—C24—C23 | 123.7 (5) |
| C7—C6—H6 | 119.7 | C25—C24—C15 | 118.1 (4) |
| C6—C7—C2 | 122.1 (7) | C23—C24—C15 | 118.1 (4) |
| C6—C7—C12' | 130.8 (7) | C24—C25—C26 | 118.6 (5) |
| C2—C7—C12' | 107.1 (5) | C24—C25—H25 | 120.7 |
| C6—C7—H7A | 119.0 | C26—C25—H25 | 120.7 |
| C2—C7—H7A | 119.0 | C27—C26—C25 | 120.4 (5) |
| C12'—C7—H7A | 12.1 | C27—C26—H26 | 119.8 |
| C9—C8—Sn1 | 111.3 (3) | C25—C26—H26 | 119.8 |
| C9—C8—H8A | 109.4 | C26—C27—C28 | 119.8 (6) |
| Sn1—C8—H8A | 109.4 | C26—C27—H27 | 120.1 |
| C9—C8—H8B | 109.4 | C28—C27—H27 | 120.1 |
| Sn1—C8—H8B | 109.4 | C23—C28—C27 | 121.7 (6) |
| H8A—C8—H8B | 108.0 | C23—C28—H28 | 119.2 |
| C10—C9—C14 | 115.9 (5) | C27—C28—H28 | 119.2 |
| O2—Sn1—O1—Sn2 | 4.51 (11) | Sn1—C8—C9—C10 | 100.7 (5) |
| C1—Sn1—O1—Sn2 | 116.9 (2) | Sn1—C8—C9—C14 | -77.6 (5) |
| O2 ⁱ —Sn1—O1—Sn2 | -5.2 (3) | C14—C9—C10—C11 | 1.2 (8) |
| C8—Sn1—O1—Sn2 | -118.63 (17) | C8—C9—C10—C11 | -177.1 (5) |
| O2—Sn2—O1—Sn1 | -4.61 (11) | C14—C9—C10—C13 | -176.6 (4) |
| C15—Sn2—O1—Sn1 | -121.91 (19) | C8—C9—C10—C13 | 5.0 (7) |
| C22—Sn2—O1—Sn1 | 105.78 (19) | C9—C10—C11—C12 | -0.5 (9) |
| C11—Sn2—O1—Sn1 | -3.5 (4) | C13—C10—C11—C12 | 177.4 (5) |
| C15—Sn2—O2—Sn1 | 82.0 (2) | C10—C11—C12—C13 | -1.2 (10) |
| C22—Sn2—O2—Sn1 | -74.7 (2) | C11—C12—C13—C14 | 2.0 (11) |
| O1—Sn2—O2—Sn1 | 5.17 (13) | C12—C13—C14—C9 | -1.3 (10) |
| C11—Sn2—O2—Sn1 | -174.49 (13) | C10—C9—C14—C13 | -0.3 (8) |
| C15—Sn2—O2—Sn1 ⁱ | -114.1 (3) | C8—C9—C14—C13 | 178.1 (6) |
| C22—Sn2—O2—Sn1 ⁱ | 89.3 (3) | O2—Sn2—C15—C16 | 118.1 (4) |
| O1—Sn2—O2—Sn1 ⁱ | 169.1 (3) | C22—Sn2—C15—C16 | -92.2 (5) |
| C11—Sn2—O2—Sn1 ⁱ | -10.5 (2) | O1—Sn2—C15—C16 | -173.6 (4) |
| C1—Sn1—O2—Sn2 | -100.2 (2) | C11—Sn2—C15—C16 | 22.1 (5) |
| O2 ⁱ —Sn1—O2—Sn2 | 169.2 (2) | Sn2—C15—C16—C17 | -83.9 (6) |
| C8—Sn1—O2—Sn2 | 81.0 (2) | Sn2—C15—C16—C21 | 98.5 (5) |
| O1—Sn1—O2—Sn2 | -5.41 (13) | C21—C16—C17—C18 | -2.0 (8) |
| C1—Sn1—O2—Sn1 ⁱ | 90.6 (2) | C15—C16—C17—C18 | -179.7 (5) |
| O2 ⁱ —Sn1—O2—Sn1 ⁱ | 0.000 (1) | C21—C16—C17—C14 | 176.0 (4) |
| C8—Sn1—O2—Sn1 ⁱ | -88.2 (2) | C15—C16—C17—C14 | -1.6 (7) |
| O1—Sn1—O2—Sn1 ⁱ | -174.57 (16) | C16—C17—C18—C19 | 1.9 (9) |
| O2—Sn1—C1—C2 | 55.6 (6) | C14—C17—C18—C19 | -176.2 (5) |
| O2 ⁱ —Sn1—C1—C2 | 130.8 (5) | C17—C18—C19—C20 | -0.2 (10) |
| C8—Sn1—C1—C2 | -125.5 (5) | C18—C19—C20—C21 | -1.1 (10) |
| O1—Sn1—C1—C2 | -22.0 (6) | C19—C20—C21—C16 | 0.9 (9) |
| Sn1—C1—C2—C7 | -94.6 (6) | C17—C16—C21—C20 | 0.6 (8) |
| Sn1—C1—C2—C3 | 85.5 (6) | C15—C16—C21—C20 | 178.4 (5) |

supplementary materials

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|----------------------------|------------|-----------------|------------|
| C7—C2—C3—C4 | -1.9 (8) | O2—Sn2—C22—C23 | -116.2 (4) |
| C1—C2—C3—C4 | 178.0 (5) | C15—Sn2—C22—C23 | 92.7 (5) |
| C7—C2—C3—C12 | 176.7 (4) | O1—Sn2—C22—C23 | 173.9 (4) |
| C1—C2—C3—C12 | -3.4 (7) | C11—Sn2—C22—C23 | -22.8 (4) |
| C2—C3—C4—C5 | 1.3 (9) | Sn2—C22—C23—C24 | -74.9 (6) |
| C12—C3—C4—C5 | -177.2 (5) | Sn2—C22—C23—C28 | 107.0 (5) |
| C3—C4—C5—C6 | 0.7 (9) | C28—C23—C24—C25 | 0.8 (8) |
| C4—C5—C6—C7 | -2.0 (10) | C22—C23—C24—C25 | -177.4 (5) |
| C5—C6—C7—C2 | 1.3 (9) | C28—C23—C24—C15 | -178.4 (4) |
| C5—C6—C7—C12' | 177.9 (6) | C22—C23—C24—C15 | 3.5 (7) |
| C3—C2—C7—C6 | 0.6 (8) | C23—C24—C25—C26 | 0.2 (9) |
| C1—C2—C7—C6 | -179.3 (5) | C15—C24—C25—C26 | 179.3 (4) |
| C3—C2—C7—C12' | -176.7 (4) | C24—C25—C26—C27 | -0.8 (9) |
| C1—C2—C7—C12' | 3.3 (7) | C25—C26—C27—C28 | 0.3 (10) |
| O2—Sn1—C8—C9 | -131.3 (3) | C24—C23—C28—C27 | -1.3 (8) |
| C1—Sn1—C8—C9 | 50.0 (5) | C22—C23—C28—C27 | 176.9 (5) |
| O2 ⁱ —Sn1—C8—C9 | 153.6 (4) | C26—C27—C28—C23 | 0.7 (10) |
| O1—Sn1—C8—C9 | -56.2 (4) | | |

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

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

| | | | | |
|--------------------|-------|-------------|-------------|---------------|
| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
| O1—H1 \cdots C12 | 0.86 | 2.80 | 3.386 (4) | 127 |

Fig. 1

