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Tetrakis(phenylethynyl)tin(IV)

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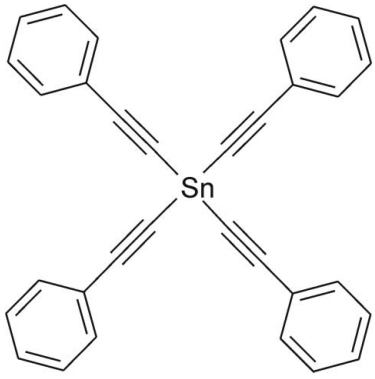
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.011 Å; R factor = 0.049; wR factor = 0.078; data-to-parameter ratio = 19.2.

The asymmetric unit of the crystal structure of the title compound, $[Sn(C_8H_5)_4]$, consists of one fourth of a discrete tin complex and one half of another which both possess nearly ideal tetrahedral symmetry; the site symmetries of the two Sn atoms are $\overline{4}$ and 2. The bond angles at all acetylide C atoms are almost linear. The Sn—C distances [2.076 (6) and 2.065 (6)–2.069 (6) Å in the two complexes) are short when compared to the sum of the covalent radii of C and Sn (2.177 Å), but consistent with another tetrakis(alkynyl)tin complex. The acetylenic bond distances [1.196 (7) and 1.183 (7)–1.207 (7) Å] are consistent with a triple C≡C bond. Therefore, despite the short Sn—C distances, the ligands are mainly σ-bonded to the metal. In the solid state, these complexes form a three-dimensional network *via* agostic C—H interactions as a phenyl proton in the *ortho* position interacts with the acetylenic carbon in the α position to the tin center.

Related literature

For related literature, see: Chen & Woo (1998); Dallaire *et al.* (1993); Jousseaume *et al.* (1998); Lahcini *et al.* (2004); Touchard *et al.* (1997); Kottke & Stalke (1993).



Experimental

Crystal data

$[Sn(C_8H_5)_4]$
M_r = 523.17
Tetragonal, $I\overline{4}$
a = 13.689 (1) Å
c = 20.098 (1) Å
V = 3766.1 (4) Å^3
Z = 6
Mo $K\alpha$ radiation
μ = 1.03 mm^{-1}
T = 173 (2) K
0.30 × 0.10 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.747, T_{max} = 0.904
9860 measured reflections
4311 independent reflections
2474 reflections with $I > 2\sigma(I)$
R_{int} = 0.070

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.078
S = 0.93
4311 reflections
224 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}
Absolute structure: Flack (1983), 2075 Friedel pairs
Flack parameter: 0.00 (3)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C28—H28A···C1	0.95	2.92	3.869 (9)	174
C18—H18A···C11^{i}	0.95	2.89	3.736 (11)	149
C8—H8A···C21^{ii}	0.95	2.85	3.795 (9)	171

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

Data collection: *COLLECT* (Nonius, 2002); cell refinement: *COLLECT*; data reduction: *COLLECT*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2532).

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supplementary materials

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Tetrakis(phenylethynyl)tin(IV)

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Comment

There has been much recent interest in tetrakis(alkynyl)tin(IV) as new precursor for preparation of tin-alkoxide and sol-gel chemistry for the preparation of tin-oxide (Jousseaume *et al.*, 1998). Recently, we demonstrated that tetrakis(phenylethynyl)tin(IV) is an efficient initiator for ring-opening polymerization of lactide and ε-caprolactone providing high activity and high molar mass polymers (Lahcini *et al.*, 2004). Here, we describe the crystal structure of tetrakis(phenylethynyl)tin. It crystallized in a tetragonal space group $I\bar{4}$, which reflects high symmetry of the molecule. The asymmetric unit cell consists of one fourth of a discrete tin complex (labeled as a Sn1 in Fig. 1) and one half of another one (Sn2) which both posses nearly ideal tetrahedral symmetry. The Sn(1)—C(1)—C(2) (176.5 (5)°) and C(1)—C(2)—C(3) (176.0 (7)°) angles in Sn1 and the Sn(2)—C(11)—C(12) (171.1 (5)°) and C(11)—C(12)—C(13) (178.0 (8)°) as well as the Sn(2)—C(21)—C(22) (177.4 (6)°) and C(21)—C(22)—C(23) (176.2 (8)°) angles in Sn2 illustrate a rather linear coordination of the acetylides on the Sn centers. The Sn—C distances (2.076 Å in Sn1 and 2.065–2.069 Å in Sn2) are short when compared to the sum of the covalent radii of C and Sn (2.177 Å), but coherent with another tetrakis(alkynyl)Sn complex, Me_3Si—C≡C—Sn (2.067 Å) (Dallaire *et al.*, 1993). The acetylenic bond distances (1.196 (7) Å in Sn1 and 1.183 (7)–1.207 (7) Å in Sn2) are consistent with a triple C≡C bond and comparable to previously reported phenylethynyl complexes, *e.g. trans*-[(NH_3)Ru(C≡CPh)$(Ph_2PCH_2CH_2PPH_2)_2$] (1.187 (7) Å) (Touchard *et al.*, 1997) and amidotin porphyrin (TTP)Sn$(C{\equiv}CPh)_2$ (1.197 (3) Å) (Chen & Woo, 1998). Therefore, despite of the short Sn—C distances, the ligands are mainly σ-bonded to the metal. In the solid state these complexes form a three-dimensional network *via* agostic C—H interactions as illustrated in Fig. 1; a phenyl proton in *ortho* position interacts with the acetylenic carbon in α position to the tin center (see table of hydrogen bonds).

Experimental

The title compound was synthesized according to a published procedure (Dallaire *et al.*, 1993). Treatment of tin tetrachloride with 4 equivalents of phenyllithium in toluene led to a corresponding tetrakis(alkynyl)tin(IV). Crystals suitable for solid state structure determination were obtained by recrystallization from toluene.

Refinement

Crystal selected for the X-ray measurement at 120 K was mounted on a glass fibre using the oil drop method (Kottke & Stalke, 1993). All H atoms were introduced in their calculated positions (C—H = 0.95 Å, U_{iso}=1.2 times the U_{eq} of the carrier atom) and refined with fixed geometry with respect to their carrier atoms.

Figures

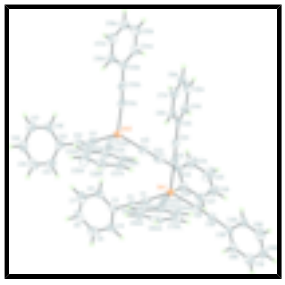


Fig. 1. A view of tetrakis(phenylethynyl)tin(IV), showing the atom-labelling scheme. Thermal ellipsoids are depicted at 50% propability level. Atoms C11A—C18A and C21A—C28A are generated with (−*x*,-*y*,*z*) and atoms C1AA—C8AA and C1B—C8B with (*x*,-*y*,-*z*) symmetry operator.

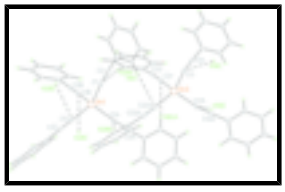


Fig. 2. Intermolecular agostic interactions in the structure of tetrakis(phenylethynyl)tin(IV) are shown as dotted lines. These distances are close to the sum of van der Waals radius of carbon and hydrogen atoms, namely C1—H28A 2.923 Å, C11—H18A (*y*,-*x*,1 − *z*) 2.888 Å and C21—H8A (−*x*,-*y*,*z*) 2.853 Å.

Tetrakis(phenylethynyl)tin(IV)

Crystal data

$[Sn(C_8H_5)_4]$	$Z = 6$
$M_r = 523.17$	$F_{000} = 1572$
Tetragonal, $I\bar{4}$	$D_x = 1.384$ Mg m^{-3}
Hall symbol: I -4	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 13.689$ (1) Å	Cell parameters from 9860 reflections
$b = 13.689$ (1) Å	$\theta = 3.4$–27.6º
$c = 20.098$ (1) Å	$\mu = 1.03$ mm^{-1}
$\alpha = 90$º	$T = 173$ (2) K
$\beta = 90$º	Needle, colourless
$\gamma = 90$º	0.30 × 0.10 × 0.10 mm
$V = 3766.1$ (4) Å^3	

Data collection

Nonius KappaCCD diffractometer	4311 independent reflections
Radiation source: fine-focus sealed tube	2474 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.070$
$T = 173(2)$ K	$\theta_{max} = 27.6$º
φ and ω scans	$\theta_{min} = 3.4$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -15 \rightarrow 17$
$T_{min} = 0.747$, $T_{max} = 0.904$	$k = -17 \rightarrow 10$
9860 measured reflections	$l = -25 \rightarrow 17$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.01P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.078$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.93$	$\Delta\rho_{max} = 0.75$ e Å^{-3}
4311 reflections	$\Delta\rho_{min} = -0.78$ e Å^{-3}
224 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 2075 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.00 (3)

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 $F^2 > 2$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	0.0000	0.0000	0.0000	0.02556 (18)
C1	0.1148 (4)	0.0423 (4)	0.0610 (2)	0.0315 (16)
C2	0.1773 (5)	0.0677 (4)	0.0988 (3)	0.0268 (15)
C3	0.2494 (6)	0.1040 (7)	0.1469 (5)	0.028 (2)
C4	0.3493 (5)	0.0952 (5)	0.1299 (3)	0.0392 (16)
H4A	0.3687	0.0664	0.0890	0.047*
C5	0.4185 (7)	0.1299 (7)	0.1749 (4)	0.049 (2)
H5A	0.4860	0.1278	0.1640	0.058*
C6	0.3886 (6)	0.1674 (5)	0.2356 (3)	0.0466 (19)
H6A	0.4361	0.1904	0.2664	0.056*
C7	0.2913 (6)	0.1719 (5)	0.2520 (3)	0.0474 (18)
H7A	0.2712	0.1975	0.2938	0.057*
C8	0.2228 (5)	0.1384 (5)	0.2065 (3)	0.0328 (17)
H8A	0.1555	0.1400	0.2180	0.039*
Sn2	0.0000	0.0000	0.312944 (19)	0.03048 (15)
C11	0.1112 (4)	0.0463 (4)	0.3751 (3)	0.0328 (15)
C12	0.1652 (5)	0.0739 (4)	0.4170 (3)	0.0345 (16)

C13	0.2279 (7)	0.1074 (7)	0.4695 (5)	0.033 (3)
C14	0.3267 (6)	0.1345 (5)	0.4593 (3)	0.0381 (19)
H14A	0.3544	0.1289	0.4161	0.046*
C15	0.3827 (5)	0.1684 (5)	0.5105 (5)	0.048 (2)
H15A	0.4491	0.1853	0.5027	0.058*
C16	0.3428 (5)	0.1786 (5)	0.5744 (3)	0.0395 (17)
H16A	0.3823	0.2022	0.6098	0.047*
C17	0.2456 (5)	0.1544 (5)	0.5862 (3)	0.0458 (19)
H17A	0.2175	0.1623	0.6291	0.055*
C18	0.1915 (7)	0.1186 (7)	0.5338 (4)	0.039 (2)
H18A	0.1256	0.1005	0.5419	0.047*
C21	0.0450 (4)	−0.1128 (5)	0.2520 (3)	0.0374 (17)
C22	0.0675 (5)	−0.1793 (5)	0.2157 (3)	0.0389 (17)
C23	0.0911 (7)	−0.2566 (7)	0.1682 (4)	0.034 (2)
C24	0.0938 (6)	−0.3541 (6)	0.1889 (4)	0.072 (3)
H24A	0.0782	−0.3718	0.2333	0.086*
C25	0.1202 (9)	−0.4245 (7)	0.1420 (4)	0.082 (4)
H25A	0.1194	−0.4915	0.1543	0.098*
C26	0.1471 (5)	−0.3998 (5)	0.0790 (3)	0.050 (2)
H26A	0.1649	−0.4495	0.0483	0.060*
C27	0.1488 (4)	−0.3049 (5)	0.0597 (3)	0.0363 (16)
H27A	0.1680	−0.2878	0.0158	0.044*
C28	0.1220 (5)	−0.2327 (5)	0.1051 (3)	0.0315 (17)
H28A	0.1252	−0.1660	0.0923	0.038*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0240 (3)	0.0240 (3)	0.0287 (4)	0.000	0.000	0.000
C1	0.032 (4)	0.039 (4)	0.024 (4)	−0.007 (3)	−0.001 (3)	0.000 (3)
C2	0.030 (4)	0.025 (4)	0.025 (4)	0.000 (3)	0.001 (3)	−0.001 (3)
C3	0.020 (5)	0.028 (5)	0.037 (6)	0.002 (4)	−0.001 (4)	0.017 (4)
C4	0.027 (4)	0.051 (5)	0.040 (4)	0.003 (4)	0.004 (4)	−0.001 (4)
C5	0.040 (5)	0.060 (6)	0.046 (6)	0.000 (4)	−0.001 (4)	0.014 (4)
C6	0.050 (5)	0.030 (4)	0.060 (5)	−0.012 (4)	−0.025 (4)	0.008 (3)
C7	0.059 (6)	0.036 (4)	0.046 (4)	−0.004 (4)	−0.009 (4)	0.003 (3)
C8	0.027 (4)	0.039 (5)	0.033 (4)	−0.003 (4)	−0.004 (3)	0.005 (3)
Sn2	0.0280 (8)	0.0333 (8)	0.0302 (3)	0.0035 (9)	0.000	0.000
C11	0.033 (4)	0.045 (4)	0.020 (3)	−0.004 (3)	0.003 (3)	0.009 (3)
C12	0.034 (5)	0.037 (4)	0.032 (4)	0.007 (3)	0.003 (3)	0.007 (3)
C13	0.037 (6)	0.021 (5)	0.043 (5)	0.005 (4)	0.001 (4)	−0.002 (3)
C14	0.040 (6)	0.036 (5)	0.039 (4)	0.007 (4)	0.005 (4)	0.000 (3)
C15	0.038 (4)	0.042 (4)	0.065 (7)	−0.009 (3)	−0.005 (5)	0.000 (5)
C16	0.043 (5)	0.031 (4)	0.045 (4)	0.007 (4)	−0.011 (4)	−0.006 (3)
C17	0.062 (6)	0.038 (5)	0.037 (4)	−0.004 (4)	0.004 (4)	−0.002 (3)
C18	0.034 (6)	0.028 (5)	0.055 (6)	0.000 (5)	−0.005 (4)	−0.004 (3)
C21	0.035 (5)	0.043 (5)	0.034 (4)	0.004 (4)	−0.003 (3)	−0.001 (3)
C22	0.032 (5)	0.049 (5)	0.036 (4)	0.009 (4)	0.003 (3)	0.009 (3)

C23	0.016 (4)	0.043 (6)	0.044 (7)	0.002 (4)	0.009 (3)	−0.002 (4)
C24	0.114 (8)	0.043 (6)	0.058 (6)	0.010 (5)	0.029 (6)	0.005 (5)
C25	0.153 (10)	0.032 (6)	0.061 (7)	0.008 (6)	0.031 (6)	0.002 (5)
C26	0.070 (6)	0.031 (5)	0.050 (5)	0.008 (4)	0.011 (4)	−0.003 (3)
C27	0.025 (4)	0.054 (5)	0.030 (4)	0.005 (3)	0.001 (3)	0.005 (3)
C28	0.030 (4)	0.029 (5)	0.035 (4)	0.010 (3)	−0.006 (3)	0.000 (3)

Geometric parameters (Å, °)

Sn1—C1	2.076 (6)	C13—C14	1.417 (11)
Sn1—C1^{i}	2.076 (6)	C14—C15	1.364 (10)
Sn1—C1^{ii}	2.076 (6)	C14—H14A	0.9500
Sn1—C1^{iii}	2.076 (6)	C15—C16	1.404 (12)
C1—C2	1.196 (7)	C15—H15A	0.9500
C2—C3	1.467 (10)	C16—C17	1.391 (9)
C3—C8	1.339 (10)	C16—H16A	0.9500
C3—C4	1.415 (10)	C17—C18	1.379 (10)
C4—C5	1.393 (10)	C17—H17A	0.9500
C4—H4A	0.9500	C18—H18A	0.9500
C5—C6	1.387 (9)	C21—C22	1.207 (7)
C5—H5A	0.9500	C22—C23	1.461 (11)
C6—C7	1.374 (8)	C23—C28	1.377 (10)
C6—H6A	0.9500	C23—C24	1.398 (12)
C7—C8	1.387 (8)	C24—C25	1.396 (10)
C7—H7A	0.9500	C24—H24A	0.9500
C8—H8A	0.9500	C25—C26	1.360 (9)
Sn2—C21	2.065 (6)	C25—H25A	0.9500
Sn2—C21^{ii}	2.065 (6)	C26—C27	1.356 (8)
Sn2—C11	2.069 (6)	C26—H26A	0.9500
Sn2—C11^{ii}	2.069 (6)	C27—C28	1.394 (8)
C11—C12	1.183 (7)	C27—H27A	0.9500
C12—C13	1.435 (10)	C28—H28A	0.9500
C13—C18	1.393 (8)		
C1—Sn1—C1^{i}	110.43 (15)	C14—C13—C12	123.3 (8)
C1—Sn1—C1^{ii}	107.6 (3)	C15—C14—C13	121.1 (7)
C1^{i}—Sn1—C1^{ii}	110.43 (15)	C15—C14—H14A	119.4
C1—Sn1—C1^{iii}	110.43 (15)	C13—C14—H14A	119.4
C1^{i}—Sn1—C1^{iii}	107.6 (3)	C14—C15—C16	120.4 (7)
C1^{ii}—Sn1—C1^{iii}	110.43 (15)	C14—C15—H15A	119.8
C2—C1—Sn1	176.5 (5)	C16—C15—H15A	119.8
C1—C2—C3	176.0 (7)	C17—C16—C15	120.3 (6)
C8—C3—C4	120.5 (8)	C17—C16—H16A	119.9
C8—C3—C2	121.8 (8)	C15—C16—H16A	119.9
C4—C3—C2	117.5 (8)	C18—C17—C16	118.0 (7)
C5—C4—C3	118.2 (8)	C18—C17—H17A	121.0
C5—C4—H4A	120.9	C16—C17—H17A	121.0
C3—C4—H4A	120.9	C17—C18—C13	123.7 (9)

C6—C5—C4	119.8 (8)	C17—C18—H18A	118.1
C6—C5—H5A	120.1	C13—C18—H18A	118.1
C4—C5—H5A	120.1	C22—C21—Sn2	177.4 (6)
C7—C6—C5	121.0 (7)	C21—C22—C23	176.2 (8)
C7—C6—H6A	119.5	C28—C23—C24	119.5 (9)
C5—C6—H6A	119.5	C28—C23—C22	119.8 (8)
C6—C7—C8	118.8 (6)	C24—C23—C22	120.2 (8)
C6—C7—H7A	120.6	C25—C24—C23	117.7 (9)
C8—C7—H7A	120.6	C25—C24—H24A	121.1
C3—C8—C7	121.6 (7)	C23—C24—H24A	121.1
C3—C8—H8A	119.2	C26—C25—C24	121.8 (9)
C7—C8—H8A	119.2	C26—C25—H25A	119.1
C21—Sn2—C21^{ii}	107.2 (3)	C24—C25—H25A	119.1
C21—Sn2—C11	111.6 (2)	C27—C26—C25	120.6 (7)
C21^{ii}—Sn2—C11	110.4 (2)	C27—C26—H26A	119.7
C21—Sn2—C11^{ii}	110.4 (2)	C25—C26—H26A	119.7
C21^{ii}—Sn2—C11^{ii}	111.6 (2)	C26—C27—C28	119.1 (6)
C11—Sn2—C11^{ii}	105.7 (3)	C26—C27—H27A	120.4
C12—C11—Sn2	171.1 (5)	C28—C27—H27A	120.4
C11—C12—C13	178.0 (8)	C23—C28—C27	121.0 (7)
C18—C13—C14	116.6 (8)	C23—C28—H28A	119.5
C18—C13—C12	120.1 (9)	C27—C28—H28A	119.5
C1^{i}—Sn1—C1—C2	−145 (9)	C12—C13—C14—C15	178.2 (8)
C1^{ii}—Sn1—C1—C2	−24 (9)	C13—C14—C15—C16	−1.0 (11)
C1^{iii}—Sn1—C1—C2	97 (9)	C14—C15—C16—C17	−0.2 (10)
Sn1—C1—C2—C3	−37 (17)	C15—C16—C17—C18	1.4 (10)
C1—C2—C3—C8	34 (11)	C16—C17—C18—C13	−1.5 (13)
C1—C2—C3—C4	−150 (10)	C14—C13—C18—C17	0.4 (16)
C8—C3—C4—C5	−4.6 (12)	C12—C13—C18—C17	−177.0 (7)
C2—C3—C4—C5	179.6 (7)	C21^{ii}—Sn2—C21—C22	−71 (13)
C3—C4—C5—C6	3.0 (11)	C11—Sn2—C21—C22	168 (13)
C4—C5—C6—C7	−0.7 (11)	C11^{ii}—Sn2—C21—C22	51 (13)
C5—C6—C7—C8	−0.2 (10)	Sn2—C21—C22—C23	53 (21)
C4—C3—C8—C7	3.8 (12)	C21—C22—C23—C28	45 (12)
C2—C3—C8—C7	179.5 (7)	C21—C22—C23—C24	−142 (11)
C6—C7—C8—C3	−1.4 (10)	C28—C23—C24—C25	−5.4 (14)
C21—Sn2—C11—C12	−141 (3)	C22—C23—C24—C25	−177.7 (9)
C21^{ii}—Sn2—C11—C12	100 (3)	C23—C24—C25—C26	3.1 (16)
C11^{ii}—Sn2—C11—C12	−21 (3)	C24—C25—C26—C27	−0.2 (15)
Sn2—C11—C12—C13	2(23)	C25—C26—C27—C28	−0.4 (11)
C11—C12—C13—C18	4(21)	C24—C23—C28—C27	5.1 (13)
C11—C12—C13—C14	−173 (100)	C22—C23—C28—C27	177.4 (6)
C18—C13—C14—C15	0.9 (14)	C26—C27—C28—C23	−2.1 (10)

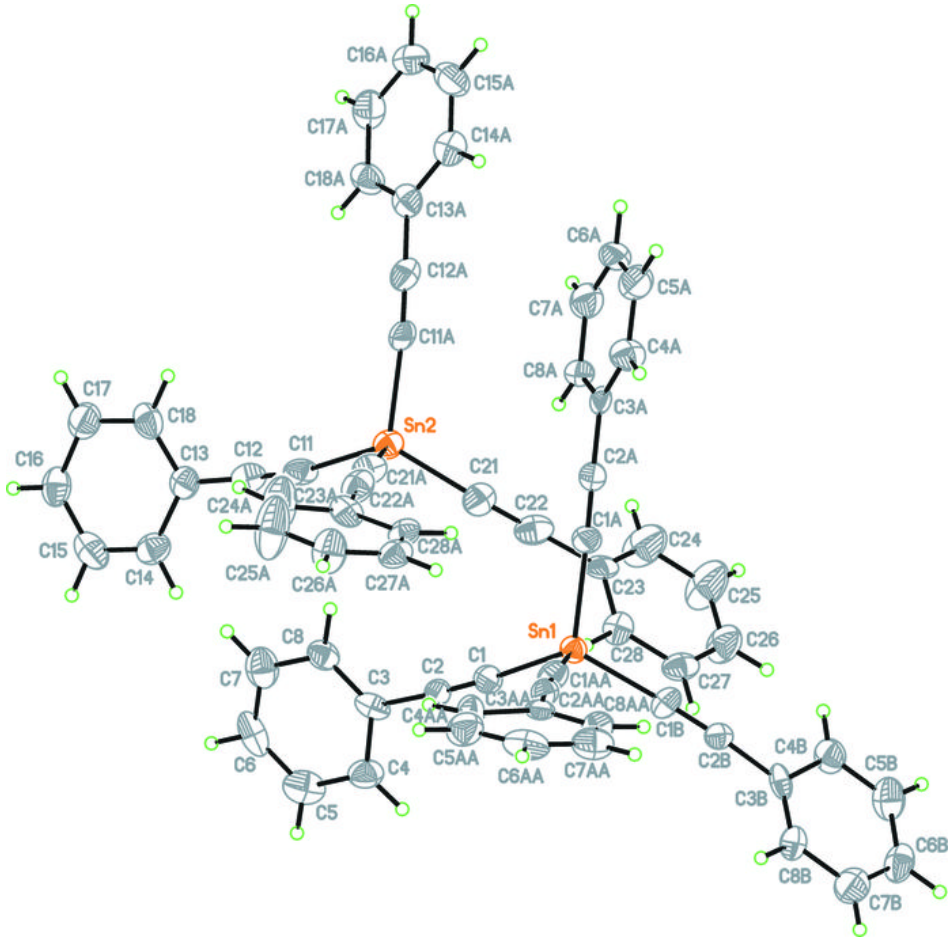
Symmetry codes: (i) *y*, −*x*, −*z*; (ii) −*x*, −*y*, *z*; (iii) −*y*, *x*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C28—H28A···C1	0.95	2.92	3.869 (9)	174
C18—H18A···C11^{iv}	0.95	2.89	3.736 (11)	149
C8—H8A···C21^{ii}	0.95	2.85	3.795 (9)	171

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

Fig. 1


C16A
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C17A
C14A
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C13A
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C11A
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C5A
C7A
C4A
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C3A
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C13
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C2
C1
C1AA
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C2AA
C8AA
C27
C1B
C4AA
C5AA
C6AA
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C4B
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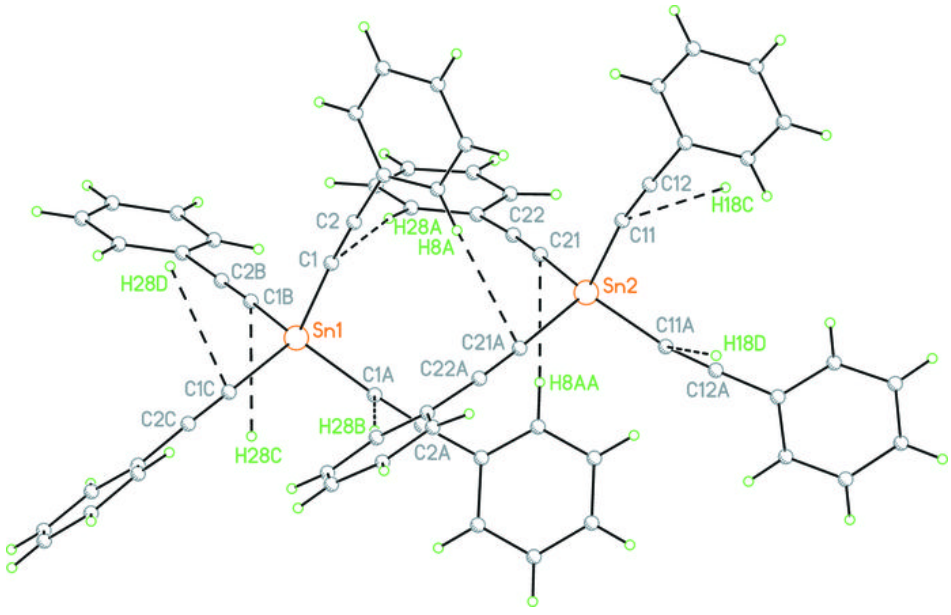
C6
C4
C5
C3B
C6B
C8B
C7B

Fig. 2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C2
H28A
C22
H8A
C21
C11
C1
Sn2
H28D
C2B
C1B
Sn1
C11A
H18D
C21A
C22A
H8AA
C1A
C12A
C1C
C2C
H28B
C2A
H28C