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Tetrakis[2-(dimethylaminomethyl)phenyl]-1κC,2κC,3κC,4κC-hexa-μ-sulfido-1:2$\kappa^4 S$:S;1,4$\kappa^2 S$:S;2:3$\kappa^2 S$:S;3:4$\kappa^4 S$:S-tetratin(IV) chloroform solvate

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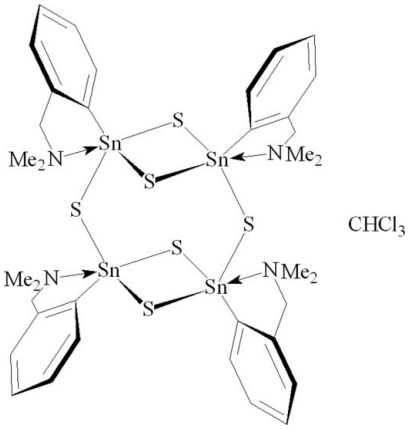
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.009 Å; disorder in solvent or counterion; R factor = 0.045; wR factor = 0.085; data-to-parameter ratio = 16.3.

The title compound, $[Sn_4(C_9H_{12}N)_4S_6]\cdot CHCl_3$, consists of four [2-($Me_2NCH_2$)$C_6H_4$]Sn units bridged by six S atoms along with a disordered solvent molecule. The cage-like structure has two four-membered Sn_2S_2 rings linked by two S atoms in an Sn_4S_6 skeleton. The asymmetry of the Sn—S bonds in the four-membered rings is the result of the combined effect of the *trans* influence of the strong N→ Sn intramolecular coordination as well as the Sn—S (axial and equatorial) bonds. The Sn atoms are pentacoordinated with a (C,N)SnS_3 trigonal bipyramidal core. Owing to intermolecular H···Ph interactions, the molecules are arranged into a polymeric ribbon along the b axis of the monoclinic unit cell. The solvent Cl atoms are disordered over two positions; the site occupancies are 0.58 and 0.42.

Related literature

For related literature, see: Dörfelt *et al.* (1968); Varga *et al.* (2001, 2005, 2006).



Experimental

Crystal data

$[Sn_4(C_9H_{12}N)_4S_6]\cdot CHCl_3$
M_r = 1323.27
Monoclinic, $P2_1/c$
a = 18.3436 (16) Å
b = 12.9426 (11) Å
c = 20.5064 (17) Å
β = 95.957 (2)°
V = 4842.2 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.50 mm^{-1}
T = 297 (2) K
0.22 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SMART*; Bruker, 2000)
T_{min} = 0.592, T_{max} = 0.685
45895 measured reflections
8532 independent reflections
7847 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.085
S = 1.25
8532 reflections
523 parameters
36 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

Table 1
X—H···π-ring interactions.

Y—X···Cg	X—H	H···Cg	X···Cg	X—H···Cg
C30—H30···$Cg1^{i}$	0.93	3.23	3.98 (1)	139
C37—H37···$Cg2^{ii}$	0.98	2.87	3.61 (1)	133

Symmetry codes: (i) $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$, (ii) $1-x, 1-y, 1-z$. $Cg1$ is the centroid of the benzene ring C1–C6, $Cg2$ is the centroid of the benzene ring C28–C33.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2007).

Financial support from the National University Research Council (grant No. CEEX 63/2006) is greatly appreciated. The authors also thank the National Center for X-ray Diffraction of Cluj-Napoca for support with the solid-state structure determination.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2339).

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supplementary materials

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Tetrakis[2-(dimethylaminomethyl)phenyl]-1κC,2κC,3κC,4κC-hexa-μ-sulfido-1:2$\kappa^4 S$:S;1,4$\kappa^2 S$:S;2:3$\kappa^2 S$:S;3:4$\kappa^4 S$:S-tetratin(IV) chloroform solvate

R. A. Varga and C. Silvestru

Comment

During our work on hypercoordinated organotin(IV) compounds with the [2-(Me_2NCH_2)C_6H_4]Sn fragment (Varga *et al.*, 2001, 2005, 2006), the title compound (**I**) was isolated as chloroform solvate. It contains two four-membered Sn_2S_2 rings, with each Sn atom bearing a (*C,N*)-coordinated organic group. The rings are bridged by two S atoms in a cage structure with a Sn_4S_6 skeleton (Fig. 1). This type of structure was suggested on the basis of mass spectra as one of the two possible structures for methyltin(IV) sulfide (Dörfelt *et al.* 1968).

The two four-membered Sn_2S_2 rings are almost parallel (dihedral angle between the planes generated by Sn1S1Sn2S2 and Sn3S3Sn4S4 atoms is 5.7 Å). They are also twisted from a Sn—Sn axis (the angle between the axis through Sn1Sn2 and Sn3Sn4 is 31.7 Å, Fig.2). The distortion of the skeleton is the result of the strong N→Sn intramolecular coordination and the difference in the Sn—S bond lengths within the Sn_2S_2 rings. The asymmetry of the Sn—S—Sn bridge in the Sn_2S_2 rings [Sn1—S1 = 2.482 (2) Å, Sn1—S2 = 2.381 (2) Å, for the other bonds see Table 1] is the result of the *trans* influence of the N→Sn intramolecular coordination and the axial and equatorial positions of the S atoms bound to Sn. These values are either longer or smaller than those of the bonds bridging the four-membered rings [Sn—S range 2.416—2.422 Å].

The Sn atoms are pentacoordinated, with the N and one S atoms in axial positions and two S and the C atom from the organic group occupying the equatorial ones (Table 1).

All the (*C,N*)SnS_3 cores are distorted from the ideal geometry as a consequence of the small 'bite' of the pendant arm ligand [C1—Sn1—N1 = 73.5 (2)°, C10—Sn1—N2 = 70.9 (1)°, C19—Sn3—N3 = 74.2 (2)°, C28—Sn4—N4 = 73.6 (2)°].

The intramolecular N→Sn interaction induces planar chirality (Varga *et al.*, 2005, 2006) and both $R_{N1}R_{N2}R_{N3}R_{N4}$ and $S_{N1}S_{N2}S_{N3}S_{N4}$ isomers are present in the crystal.

Intermolecular *H*···phenyl interactions between three aromatic H atoms and phenyl rings from the neighboring molecules (H···π range 2.87–3.23 Å, see Extra Table) link isomers of the same type and the solvent molecules in a polymeric double chain (Fig. 3) along *b* axis.

Chains of different isomers alternate in crystal, with no further interactions between polymers.

Experimental

A solution of [2-(Me_2NCH_2)C_6H_4]$SnCl_3$ (0.25 g, 0.7 mmol) in CH_2Cl_2 (15 ml) was treated with an aqueous solution of Na_2S (0.41 g, 5.25 mmol, 500% excess) and the reaction was stirred for 3 h at room temperature. The organic layer was separated, the water solution was washed with dichloromethane (2x5 ml) and the combined organic phases were dried over

anhydrous Na_2SO_4. After removal of the solvent under vacuum the title compound was isolated as a white crystalline solid (0.19 g, 90%).

Refinement

All hydrogen atoms were placed in calculated positions using a riding model, with C—H = 0.93–0.97 Å and with U_{iso}= 1.5U_{eq} (C) for methyl H and U_{iso}= 1.2U_{eq} (C) for aryl H. The methyl groups were allowed to rotate but not to tip. The chloroform molecule is disordered over two orientations related by rotation about its C—H bond, with site occupancy of 42:58 for the Cl atoms. The C—Cl bonds were restrained within 0.01 Å of each other.

Figures

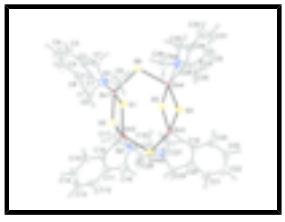

Fig. 1. : View of the title compound showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms as spheres of arbitrary radii. The solvent molecule is omitted for clarity.

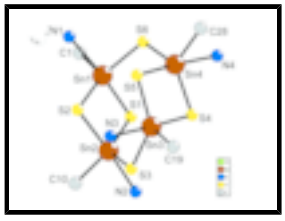

Fig. 2. : Detailed view of the inorganic skeleton of the title compound.

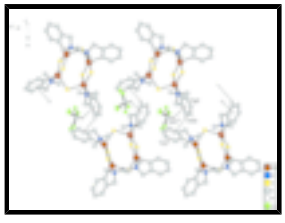

Fig. 3. : Intermolecular interactions (represented with dashed lines) in crystal structure of the title compound. Symmetry codes: (i) 1 − *x*, −1/2 + *y*, 1/2 − *z*, (ii) 1 − *x*, 1 − *y*, 1 − *z*.

Tetrakis[2-(dimethylaminomethyl)phenyl]-1κ*C*,2κ*C*,3κ*C*,4κ*C*- hexa-μ-sulfido-1:2κ^4*S*:*S*;1,4κ^2*S*:*S*;2:3κ^2*S*:*S*;3:4κ^4*S*:*S*- tetratin(IV) chloroform solvate

Crystal data

$[Sn_4(C_9H_{12}N_1)_4S_6]\cdot CHCl_3$	F_{000} = 2584
M_r = 1323.27	D_x = 1.815 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5287 reflections
a = 18.3436 (16) Å	θ = 2.2–26.0º
b = 12.9426 (11) Å	μ = 2.50 mm^{-1}
c = 20.5064 (17) Å	T = 297 (2) K
β = 95.957 (2)º	Block, colourless

V = 4842.2 (7) Å^3
Z = 4

0.22 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
T = 297(2) K
φ and ω scans
Absorption correction: multi-scan (SMART; Bruker, 2000)
T_{min} = 0.592, T_{max} = 0.685
45895 measured reflections

8532 independent reflections
7847 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 25.0º
θ_{min} = 1.9º
h = −21→21
k = −15→15
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.085
S = 1.25
8532 reflections
523 parameters
36 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0212P)^2 + 10.3311P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}
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}	Occ. (<1)
Sn1	0.26821 (2)	0.41338 (3)	0.356993 (18)	0.02986 (10)	
Sn2	0.09335 (2)	0.32210 (3)	0.347054 (18)	0.03078 (10)	

Sn4	0.33646 (2)	0.12921 (3)	0.339185 (18)	0.03016 (10)
Sn3	0.18838 (2)	0.06584 (3)	0.417327 (18)	0.03000 (10)
N1	0.3557 (3)	0.4710 (4)	0.4535 (2)	0.0386 (12)
N2	−0.0021 (3)	0.2856 (4)	0.2536 (2)	0.0424 (12)
N3	0.1607 (3)	0.0792 (4)	0.5356 (2)	0.0394 (12)
N4	0.3635 (3)	0.1102 (4)	0.2201 (2)	0.0467 (13)
S1	0.17372 (9)	0.36588 (14)	0.26650 (7)	0.0466 (4)
S2	0.18540 (8)	0.38160 (13)	0.43677 (7)	0.0398 (4)
S3	0.07148 (8)	0.15029 (12)	0.38754 (8)	0.0416 (4)
S4	0.22241 (9)	0.04969 (13)	0.30360 (7)	0.0450 (4)
S5	0.30716 (8)	0.13240 (13)	0.45431 (7)	0.0390 (4)
S6	0.36809 (8)	0.30876 (11)	0.32632 (8)	0.0367 (3)
C1	0.3035 (3)	0.5660 (4)	0.3343 (3)	0.0372 (14)
C2	0.3662 (3)	0.6021 (4)	0.3702 (3)	0.0417 (15)
C3	0.3921 (4)	0.7007 (5)	0.3580 (4)	0.060 (2)
H3	0.4351	0.7244	0.3811	0.071*
C4	0.3551 (6)	0.7616 (6)	0.3130 (4)	0.080 (3)
H4	0.3724	0.8279	0.3065	0.096*
C5	0.2928 (6)	0.7292 (6)	0.2764 (4)	0.077 (3)
H5	0.2685	0.7724	0.2450	0.093*
C6	0.2660 (4)	0.6295 (5)	0.2871 (3)	0.0534 (18)
H6	0.2236	0.6060	0.2628	0.064*
C7	0.4072 (3)	0.5336 (5)	0.4202 (3)	0.0458 (16)
H7A	0.4398	0.4886	0.3990	0.055*
H7B	0.4366	0.5755	0.4521	0.055*
C8	0.3183 (4)	0.5377 (5)	0.4981 (3)	0.0530 (17)
H8A	0.3542	0.5695	0.5293	0.079*
H8B	0.2855	0.4967	0.5209	0.079*
H8C	0.2911	0.5903	0.4732	0.079*
C9	0.3930 (4)	0.3866 (5)	0.4916 (3)	0.0581 (19)
H9A	0.4194	0.3448	0.4634	0.087*
H9B	0.3574	0.3449	0.5105	0.087*
H9C	0.4266	0.4151	0.5260	0.087*
C10	−0.0012 (3)	0.4087 (4)	0.3667 (3)	0.0309 (12)
C11	−0.0674 (3)	0.3771 (4)	0.3341 (3)	0.0374 (14)
C12	−0.1310 (3)	0.4284 (5)	0.3456 (3)	0.0506 (17)
H12	−0.1756	0.4083	0.3235	0.061*
C13	−0.1285 (4)	0.5089 (5)	0.3895 (3)	0.0531 (18)
H13	−0.1716	0.5421	0.3977	0.064*
C14	−0.0630 (4)	0.5407 (5)	0.4212 (3)	0.0487 (17)
H14	−0.0615	0.5962	0.4502	0.058*
C15	0.0006 (3)	0.4906 (4)	0.4102 (3)	0.0380 (14)
H15	0.0450	0.5118	0.4320	0.046*
C16	−0.0690 (3)	0.2874 (5)	0.2873 (3)	0.0456 (16)
H16A	−0.0730	0.2233	0.3111	0.055*
H16B	−0.1115	0.2932	0.2552	0.055*
C17	−0.0044 (4)	0.3707 (6)	0.2056 (3)	0.0543 (18)
H17A	−0.0437	0.3590	0.1717	0.082*
H17B	0.0412	0.3737	0.1867	0.082*

H17C	−0.0124	0.4349	0.2273	0.082*	
C18	0.0064 (4)	0.1873 (6)	0.2197 (4)	0.069 (2)	
H18A	−0.0322	0.1800	0.1847	0.103*	
H18B	0.0042	0.1313	0.2502	0.103*	
H18C	0.0529	0.1862	0.2021	0.103*	
C19	0.1592 (3)	−0.0858 (4)	0.4449 (3)	0.0344 (13)	
C20	0.1201 (3)	−0.0948 (5)	0.4989 (3)	0.0395 (14)	
C21	0.0988 (4)	−0.1911 (5)	0.5190 (4)	0.0545 (18)	
H21	0.0725	−0.1966	0.5552	0.065*	
C22	0.1161 (4)	−0.2791 (5)	0.4860 (4)	0.0575 (19)	
H22	0.1012	−0.3436	0.4997	0.069*	
C23	0.1555 (4)	−0.2708 (5)	0.4327 (3)	0.0518 (17)	
H23	0.1680	−0.3300	0.4107	0.062*	
C24	0.1766 (3)	−0.1755 (5)	0.4118 (3)	0.0411 (14)	
H24	0.2026	−0.1706	0.3753	0.049*	
C25	0.1010 (3)	0.0027 (5)	0.5347 (3)	0.0469 (16)	
H25A	0.0562	0.0322	0.5131	0.056*	
H25B	0.0924	−0.0144	0.5793	0.056*	
C26	0.1360 (4)	0.1810 (5)	0.5561 (3)	0.0558 (18)	
H26A	0.1240	0.1772	0.6005	0.084*	
H26B	0.0934	0.2016	0.5279	0.084*	
H26C	0.1744	0.2307	0.5533	0.084*	
C27	0.2239 (4)	0.0454 (5)	0.5806 (3)	0.0537 (18)	
H27A	0.2621	0.0962	0.5815	0.081*	
H27B	0.2417	−0.0194	0.5659	0.081*	
H27C	0.2092	0.0373	0.6239	0.081*	
C28	0.4388 (3)	0.0493 (4)	0.3416 (3)	0.0372 (14)	
C29	0.4755 (3)	0.0569 (5)	0.2856 (3)	0.0465 (16)	
C30	0.5415 (4)	0.0064 (7)	0.2849 (4)	0.072 (2)	
H30	0.5658	0.0092	0.2473	0.087*	
C31	0.5718 (4)	−0.0471 (7)	0.3373 (5)	0.082 (3)	
H31	0.6172	−0.0784	0.3357	0.098*	
C32	0.5369 (4)	−0.0561 (6)	0.3930 (5)	0.074 (2)	
H32	0.5577	−0.0938	0.4288	0.089*	
C33	0.4685 (4)	−0.0066 (5)	0.3947 (4)	0.0518 (17)	
H33	0.4435	−0.0120	0.4317	0.062*	
C34	0.4429 (4)	0.1218 (6)	0.2285 (3)	0.0556 (19)	
H34A	0.4554	0.1938	0.2364	0.067*	
H34B	0.4631	0.1003	0.1888	0.067*	
C35	0.3432 (4)	0.0075 (5)	0.1938 (3)	0.0557 (18)	
H35A	0.3571	0.0015	0.1501	0.084*	
H35B	0.2912	−0.0017	0.1930	0.084*	
H35C	0.3680	−0.0445	0.2212	0.084*	
C36	0.3280 (5)	0.1901 (6)	0.1756 (3)	0.069 (2)	
H36A	0.3413	0.2575	0.1924	0.103*	
H36B	0.2757	0.1821	0.1729	0.103*	
H36C	0.3440	0.1823	0.1328	0.103*	
Cl1A	0.2869 (4)	0.7495 (10)	0.6065 (6)	0.133 (6)	0.42 (2)
Cl2B	0.4358 (4)	0.7223 (7)	0.6359 (7)	0.091 (3)	0.58 (2)

Cl3B	0.3910 (9)	0.8116 (11)	0.5126 (3)	0.244 (9)	0.58 (2)
C37	0.3710 (3)	0.8011 (5)	0.5928 (3)	0.085 (3)	
H37	0.3788	0.8640	0.6191	0.102*	
Cl1B	0.2842 (2)	0.7498 (6)	0.5950 (4)	0.102 (3)	0.58 (2)
Cl3A	0.3707 (5)	0.8341 (11)	0.5111 (3)	0.104 (4)	0.42 (2)
Cl2A	0.4411 (5)	0.7160 (11)	0.6163 (8)	0.120 (6)	0.42 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0271 (2)	0.0308 (2)	0.0321 (2)	−0.00056 (16)	0.00546 (16)	0.00052 (16)
Sn2	0.0241 (2)	0.0353 (2)	0.0328 (2)	0.00175 (16)	0.00235 (16)	−0.00107 (17)
Sn4	0.0287 (2)	0.0305 (2)	0.0328 (2)	−0.00044 (16)	0.01042 (16)	0.00009 (16)
Sn3	0.0254 (2)	0.0303 (2)	0.0353 (2)	−0.00136 (16)	0.00764 (16)	0.00113 (16)
N1	0.039 (3)	0.040 (3)	0.037 (3)	−0.008 (2)	0.001 (2)	−0.001 (2)
N2	0.036 (3)	0.051 (3)	0.040 (3)	0.003 (2)	−0.001 (2)	−0.010 (2)
N3	0.043 (3)	0.038 (3)	0.040 (3)	0.000 (2)	0.016 (2)	−0.003 (2)
N4	0.060 (4)	0.045 (3)	0.038 (3)	−0.011 (3)	0.019 (3)	−0.001 (2)
S1	0.0388 (9)	0.0720 (12)	0.0291 (8)	−0.0096 (8)	0.0040 (7)	−0.0018 (8)
S2	0.0299 (8)	0.0602 (10)	0.0295 (8)	−0.0075 (7)	0.0041 (6)	−0.0021 (7)
S3	0.0252 (8)	0.0402 (9)	0.0597 (10)	−0.0007 (6)	0.0051 (7)	0.0093 (7)
S4	0.0424 (9)	0.0602 (11)	0.0330 (8)	−0.0142 (8)	0.0075 (7)	−0.0075 (7)
S5	0.0310 (8)	0.0548 (10)	0.0318 (8)	−0.0092 (7)	0.0071 (6)	−0.0024 (7)
S6	0.0333 (8)	0.0299 (8)	0.0500 (9)	−0.0019 (6)	0.0185 (7)	−0.0007 (7)
C1	0.046 (4)	0.027 (3)	0.041 (3)	0.001 (3)	0.017 (3)	0.001 (3)
C2	0.050 (4)	0.033 (3)	0.046 (4)	−0.009 (3)	0.023 (3)	−0.009 (3)
C3	0.074 (5)	0.047 (4)	0.061 (5)	−0.024 (4)	0.023 (4)	−0.010 (4)
C4	0.129 (8)	0.048 (5)	0.066 (6)	−0.013 (5)	0.026 (6)	0.012 (4)
C5	0.121 (8)	0.049 (5)	0.064 (5)	0.015 (5)	0.022 (5)	0.022 (4)
C6	0.064 (5)	0.048 (4)	0.051 (4)	0.010 (3)	0.016 (3)	0.011 (3)
C7	0.035 (3)	0.045 (4)	0.057 (4)	−0.012 (3)	0.004 (3)	−0.007 (3)
C8	0.055 (4)	0.062 (4)	0.041 (4)	−0.009 (3)	0.001 (3)	−0.009 (3)
C9	0.053 (4)	0.064 (5)	0.053 (4)	−0.006 (4)	−0.015 (3)	0.008 (4)
C10	0.027 (3)	0.031 (3)	0.035 (3)	0.005 (2)	0.001 (2)	0.005 (2)
C11	0.033 (3)	0.036 (3)	0.042 (3)	0.004 (3)	0.003 (3)	0.004 (3)
C12	0.035 (4)	0.069 (5)	0.047 (4)	0.010 (3)	0.001 (3)	0.005 (4)
C13	0.039 (4)	0.065 (5)	0.057 (4)	0.029 (3)	0.011 (3)	0.012 (4)
C14	0.065 (5)	0.044 (4)	0.039 (4)	0.018 (3)	0.015 (3)	0.000 (3)
C15	0.048 (4)	0.036 (3)	0.030 (3)	0.004 (3)	0.004 (3)	0.005 (3)
C16	0.035 (3)	0.053 (4)	0.048 (4)	−0.008 (3)	−0.002 (3)	−0.001 (3)
C17	0.050 (4)	0.075 (5)	0.036 (4)	0.002 (4)	−0.002 (3)	0.007 (3)
C18	0.076 (5)	0.064 (5)	0.062 (5)	0.005 (4)	−0.013 (4)	−0.026 (4)
C19	0.028 (3)	0.028 (3)	0.047 (4)	−0.001 (2)	0.004 (3)	0.004 (3)
C20	0.032 (3)	0.043 (4)	0.045 (4)	−0.005 (3)	0.006 (3)	0.005 (3)
C21	0.050 (4)	0.050 (4)	0.065 (5)	−0.013 (3)	0.015 (3)	0.017 (4)
C22	0.072 (5)	0.035 (4)	0.064 (5)	−0.015 (3)	0.004 (4)	0.010 (3)
C23	0.054 (4)	0.035 (4)	0.064 (5)	−0.004 (3)	−0.007 (4)	−0.002 (3)
C24	0.036 (3)	0.043 (4)	0.042 (4)	0.005 (3)	−0.004 (3)	0.000 (3)

C25	0.043 (4)	0.044 (4)	0.058 (4)	−0.003 (3)	0.026 (3)	0.004 (3)
C26	0.074 (5)	0.043 (4)	0.055 (4)	0.008 (4)	0.025 (4)	−0.010 (3)
C27	0.062 (5)	0.066 (5)	0.033 (3)	−0.004 (4)	0.005 (3)	0.002 (3)
C28	0.032 (3)	0.028 (3)	0.052 (4)	0.001 (2)	0.006 (3)	−0.009 (3)
C29	0.039 (4)	0.047 (4)	0.056 (4)	−0.002 (3)	0.020 (3)	−0.024 (3)
C30	0.049 (5)	0.085 (6)	0.085 (6)	0.007 (4)	0.017 (4)	−0.038 (5)
C31	0.048 (5)	0.084 (6)	0.111 (8)	0.027 (4)	−0.005 (5)	−0.035 (6)
C32	0.061 (5)	0.050 (5)	0.106 (7)	0.016 (4)	−0.020 (5)	−0.010 (5)
C33	0.052 (4)	0.038 (4)	0.067 (5)	−0.001 (3)	0.013 (4)	−0.003 (3)
C34	0.061 (5)	0.062 (5)	0.050 (4)	−0.013 (4)	0.034 (4)	−0.010 (4)
C35	0.079 (5)	0.053 (4)	0.036 (4)	−0.011 (4)	0.011 (3)	−0.012 (3)
C36	0.102 (6)	0.062 (5)	0.041 (4)	0.001 (4)	0.005 (4)	0.010 (4)
Cl1A	0.148 (11)	0.155 (11)	0.112 (7)	0.002 (8)	0.086 (8)	0.033 (7)
Cl2B	0.084 (4)	0.078 (4)	0.108 (6)	−0.016 (3)	−0.008 (3)	−0.019 (4)
Cl3B	0.55 (3)	0.102 (7)	0.095 (6)	−0.118 (11)	0.102 (9)	−0.011 (5)
C37	0.122 (8)	0.049 (5)	0.079 (6)	−0.003 (5)	−0.007 (6)	−0.016 (4)
Cl1B	0.066 (4)	0.122 (6)	0.108 (4)	0.036 (4)	−0.033 (4)	−0.058 (4)
Cl3A	0.107 (8)	0.111 (8)	0.094 (7)	−0.007 (5)	0.010 (4)	0.047 (6)
Cl2A	0.070 (6)	0.109 (8)	0.169 (14)	0.027 (5)	−0.056 (7)	−0.056 (7)

Geometric parameters (Å, °)

Sn1—C1	2.145 (6)	C13—H13	0.9300
Sn1—S2	2.3810 (15)	C14—C15	1.374 (8)
Sn1—S6	2.4134 (14)	C14—H14	0.9300
Sn1—S1	2.4816 (16)	C15—H15	0.9300
Sn1—N1	2.527 (5)	C16—H16A	0.9700
Sn2—C10	2.138 (5)	C16—H16B	0.9700
Sn2—S1	2.3935 (16)	C17—H17A	0.9600
Sn2—S3	2.4216 (16)	C17—H17B	0.9600
Sn2—S2	2.4869 (15)	C17—H17C	0.9600
Sn2—N2	2.503 (5)	C18—H18A	0.9600
Sn4—C28	2.139 (6)	C18—H18B	0.9600
Sn4—S4	2.3774 (16)	C18—H18C	0.9600
Sn4—S6	2.4162 (15)	C19—C20	1.386 (8)
Sn4—S5	2.4753 (15)	C19—C24	1.397 (8)
Sn4—N4	2.554 (5)	C20—C21	1.381 (8)
Sn3—C19	2.126 (5)	C20—C25	1.519 (8)
Sn3—S5	2.3919 (15)	C21—C22	1.379 (9)
Sn3—S3	2.4278 (15)	C21—H21	0.9300
Sn3—S4	2.4847 (15)	C22—C23	1.375 (9)
Sn3—N3	2.536 (5)	C22—H22	0.9300
N1—C7	1.465 (7)	C23—C24	1.375 (8)
N1—C9	1.471 (8)	C23—H23	0.9300
N1—C8	1.477 (8)	C24—H24	0.9300
N2—C18	1.465 (8)	C25—H25A	0.9700
N2—C16	1.469 (7)	C25—H25B	0.9700
N2—C17	1.474 (8)	C26—H26A	0.9600
N3—C26	1.468 (7)	C26—H26B	0.9600

N3—C27	1.472 (8)	C26—H26C	0.9600
N3—C25	1.476 (7)	C27—H27A	0.9600
N4—C34	1.455 (8)	C27—H27B	0.9600
N4—C35	1.468 (8)	C27—H27C	0.9600
N4—C36	1.484 (8)	C28—C33	1.372 (9)
C1—C2	1.381 (8)	C28—C29	1.393 (8)
C1—C6	1.396 (8)	C29—C30	1.377 (9)
C2—C3	1.393 (8)	C29—C34	1.514 (9)
C2—C7	1.498 (9)	C30—C31	1.349 (12)
C3—C4	1.343 (11)	C30—H30	0.9300
C3—H3	0.9300	C31—C32	1.370 (12)
C4—C5	1.366 (12)	C31—H31	0.9300
C4—H4	0.9300	C32—C33	1.413 (10)
C5—C6	1.406 (10)	C32—H32	0.9300
C5—H5	0.9300	C33—H33	0.9300
C6—H6	0.9300	C34—H34A	0.9700
C7—H7A	0.9700	C34—H34B	0.9700
C7—H7B	0.9700	C35—H35A	0.9600
C8—H8A	0.9600	C35—H35B	0.9600
C8—H8B	0.9600	C35—H35C	0.9600
C8—H8C	0.9600	C36—H36A	0.9600
C9—H9A	0.9600	C36—H36B	0.9600
C9—H9B	0.9600	C36—H36C	0.9600
C9—H9C	0.9600	Cl1A—C37	1.730 (6)
C10—C15	1.384 (8)	Cl2B—C37	1.736 (6)
C10—C11	1.386 (8)	Cl3B—C37	1.728 (6)
C11—C12	1.384 (8)	C37—Cl2A	1.723 (7)
C11—C16	1.505 (8)	C37—Cl3A	1.728 (6)
C12—C13	1.376 (9)	C37—Cl1B	1.729 (6)
C12—H12	0.9300	C37—H37	0.9800
C13—C14	1.369 (9)		
C1—Sn1—S2	122.44 (15)	C14—C13—H13	119.7
C1—Sn1—S6	101.89 (15)	C12—C13—H13	119.7
S2—Sn1—S6	129.63 (6)	C13—C14—C15	119.9 (6)
C1—Sn1—S1	105.62 (17)	C13—C14—H14	120.1
S2—Sn1—S1	91.44 (5)	C15—C14—H14	120.1
S6—Sn1—S1	99.00 (6)	C14—C15—C10	120.3 (6)
C1—Sn1—N1	73.5 (2)	C14—C15—H15	119.8
S2—Sn1—N1	84.93 (11)	C10—C15—H15	119.8
S6—Sn1—N1	86.11 (12)	N2—C16—C11	110.5 (5)
S1—Sn1—N1	174.88 (12)	N2—C16—H16A	109.5
C10—Sn2—S1	125.14 (15)	C11—C16—H16A	109.5
C10—Sn2—S3	104.51 (15)	N2—C16—H16B	109.5
S1—Sn2—S3	126.15 (6)	C11—C16—H16B	109.5
C10—Sn2—S2	101.53 (15)	H16A—C16—H16B	108.1
S1—Sn2—S2	91.02 (5)	N2—C17—H17A	109.5
S3—Sn2—S2	98.89 (6)	N2—C17—H17B	109.5
C10—Sn2—N2	74.15 (18)	H17A—C17—H17B	109.5
S1—Sn2—N2	87.02 (12)	N2—C17—H17C	109.5

S3—Sn2—N2	87.81 (13)	H17A—C17—H17C	109.5
S2—Sn2—N2	172.83 (13)	H17B—C17—H17C	109.5
C28—Sn4—S4	122.68 (15)	N2—C18—H18A	109.5
C28—Sn4—S6	104.33 (15)	N2—C18—H18B	109.5
S4—Sn4—S6	126.62 (6)	H18A—C18—H18B	109.5
C28—Sn4—S5	105.26 (17)	N2—C18—H18C	109.5
S4—Sn4—S5	91.64 (5)	H18A—C18—H18C	109.5
S6—Sn4—S5	99.58 (5)	H18B—C18—H18C	109.5
C28—Sn4—N4	73.6 (2)	C20—C19—C24	118.8 (5)
S4—Sn4—N4	85.24 (12)	C20—C19—Sn3	117.1 (4)
S6—Sn4—N4	85.15 (12)	C24—C19—Sn3	124.1 (4)
S5—Sn4—N4	175.26 (12)	C21—C20—C19	119.9 (6)
C19—Sn3—S5	119.64 (15)	C21—C20—C25	121.3 (6)
C19—Sn3—S3	104.01 (15)	C19—C20—C25	118.8 (5)
S5—Sn3—S3	132.02 (6)	C22—C21—C20	120.9 (6)
C19—Sn3—S4	105.44 (16)	C22—C21—H21	119.6
S5—Sn3—S4	91.07 (5)	C20—C21—H21	119.6
S3—Sn3—S4	95.92 (6)	C23—C22—C21	119.4 (6)
C19—Sn3—N3	74.23 (19)	C23—C22—H22	120.3
S5—Sn3—N3	86.46 (12)	C21—C22—H22	120.3
S3—Sn3—N3	87.17 (12)	C22—C23—C24	120.4 (6)
S4—Sn3—N3	176.87 (12)	C22—C23—H23	119.8
C7—N1—C9	111.8 (5)	C24—C23—H23	119.8
C7—N1—C8	109.2 (5)	C23—C24—C19	120.5 (6)
C9—N1—C8	108.9 (5)	C23—C24—H24	119.7
C7—N1—Sn1	100.8 (3)	C19—C24—H24	119.7
C9—N1—Sn1	114.8 (4)	N3—C25—C20	110.8 (5)
C8—N1—Sn1	111.1 (4)	N3—C25—H25A	109.5
C18—N2—C16	111.8 (5)	C20—C25—H25A	109.5
C18—N2—C17	109.3 (5)	N3—C25—H25B	109.5
C16—N2—C17	109.5 (5)	C20—C25—H25B	109.5
C18—N2—Sn2	115.2 (4)	H25A—C25—H25B	108.1
C16—N2—Sn2	100.9 (3)	N3—C26—H26A	109.5
C17—N2—Sn2	109.9 (4)	N3—C26—H26B	109.5
C26—N3—C27	109.5 (5)	H26A—C26—H26B	109.5
C26—N3—C25	110.8 (5)	N3—C26—H26C	109.5
C27—N3—C25	110.1 (5)	H26A—C26—H26C	109.5
C26—N3—Sn3	115.7 (4)	H26B—C26—H26C	109.5
C27—N3—Sn3	110.9 (3)	N3—C27—H27A	109.5
C25—N3—Sn3	99.4 (3)	N3—C27—H27B	109.5
C34—N4—C35	110.5 (5)	H27A—C27—H27B	109.5
C34—N4—C36	111.8 (5)	N3—C27—H27C	109.5
C35—N4—C36	109.1 (5)	H27A—C27—H27C	109.5
C34—N4—Sn4	99.7 (4)	H27B—C27—H27C	109.5
C35—N4—Sn4	111.8 (4)	C33—C28—C29	120.3 (6)
C36—N4—Sn4	113.8 (4)	C33—C28—Sn4	123.2 (5)
Sn2—S1—Sn1	88.57 (5)	C29—C28—Sn4	116.5 (5)
Sn1—S2—Sn2	88.73 (5)	C30—C29—C28	118.5 (7)
Sn2—S3—Sn3	109.04 (6)	C30—C29—C34	122.1 (6)

Sn4—S4—Sn3	88.53 (5)	C28—C29—C34	119.4 (5)
Sn3—S5—Sn4	88.42 (5)	C31—C30—C29	121.6 (8)
Sn1—S6—Sn4	108.29 (5)	C31—C30—H30	119.2
C2—C1—C6	119.6 (6)	C29—C30—H30	119.2
C2—C1—Sn1	116.7 (4)	C30—C31—C32	121.2 (8)
C6—C1—Sn1	123.7 (5)	C30—C31—H31	119.4
C1—C2—C3	119.7 (6)	C32—C31—H31	119.4
C1—C2—C7	119.7 (5)	C31—C32—C33	118.4 (8)
C3—C2—C7	120.6 (6)	C31—C32—H32	120.8
C4—C3—C2	120.2 (8)	C33—C32—H32	120.8
C4—C3—H3	119.9	C28—C33—C32	120.0 (7)
C2—C3—H3	119.9	C28—C33—H33	120.0
C3—C4—C5	122.1 (8)	C32—C33—H33	120.0
C3—C4—H4	118.9	N4—C34—C29	110.2 (5)
C5—C4—H4	118.9	N4—C34—H34A	109.6
C4—C5—C6	118.8 (8)	C29—C34—H34A	109.6
C4—C5—H5	120.6	N4—C34—H34B	109.6
C6—C5—H5	120.6	C29—C34—H34B	109.6
C1—C6—C5	119.6 (7)	H34A—C34—H34B	108.1
C1—C6—H6	120.2	N4—C35—H35A	109.5
C5—C6—H6	120.2	N4—C35—H35B	109.5
N1—C7—C2	110.1 (5)	H35A—C35—H35B	109.5
N1—C7—H7A	109.6	N4—C35—H35C	109.5
C2—C7—H7A	109.6	H35A—C35—H35C	109.5
N1—C7—H7B	109.6	H35B—C35—H35C	109.5
C2—C7—H7B	109.6	N4—C36—H36A	109.5
H7A—C7—H7B	108.1	N4—C36—H36B	109.5
N1—C8—H8A	109.5	H36A—C36—H36B	109.5
N1—C8—H8B	109.5	N4—C36—H36C	109.5
H8A—C8—H8B	109.5	H36A—C36—H36C	109.5
N1—C8—H8C	109.5	H36B—C36—H36C	109.5
H8A—C8—H8C	109.5	Cl2A—C37—Cl3B	95.2 (8)
H8B—C8—H8C	109.5	Cl2A—C37—Cl3A	110.9 (5)
N1—C9—H9A	109.5	Cl2A—C37—Cl1B	114.2 (7)
N1—C9—H9B	109.5	Cl3B—C37—Cl1B	110.0 (5)
H9A—C9—H9B	109.5	Cl3A—C37—Cl1B	102.1 (5)
N1—C9—H9C	109.5	Cl2A—C37—Cl1A	111.1 (5)
H9A—C9—H9C	109.5	Cl3B—C37—Cl1A	117.8 (7)
H9B—C9—H9C	109.5	Cl3A—C37—Cl1A	109.9 (5)
C15—C10—C11	119.9 (5)	Cl3B—C37—Cl2B	109.2 (5)
C15—C10—Sn2	123.9 (4)	Cl3A—C37—Cl2B	124.8 (7)
C11—C10—Sn2	116.2 (4)	Cl1B—C37—Cl2B	110.2 (4)
C12—C11—C10	119.3 (6)	Cl1A—C37—Cl2B	105.4 (6)
C12—C11—C16	121.2 (6)	Cl2A—C37—H37	108.3
C10—C11—C16	119.5 (5)	Cl3B—C37—H37	115.1
C13—C12—C11	120.2 (6)	Cl3A—C37—H37	108.3
C13—C12—H12	119.9	Cl1B—C37—H37	112.8
C11—C12—H12	119.9	Cl1A—C37—H37	108.3
C14—C13—C12	120.5 (6)	Cl2B—C37—H37	98.9

C1—Sn1—N1—C7	−34.1 (4)	C6—C1—C2—C3	−1.1 (9)
S2—Sn1—N1—C7	−160.1 (4)	Sn1—C1—C2—C3	−179.9 (5)
S6—Sn1—N1—C7	69.6 (3)	C6—C1—C2—C7	−179.1 (6)
C1—Sn1—N1—C9	−154.3 (5)	Sn1—C1—C2—C7	2.1 (7)
S2—Sn1—N1—C9	79.7 (4)	C1—C2—C3—C4	1.9 (10)
S6—Sn1—N1—C9	−50.7 (4)	C7—C2—C3—C4	180.0 (7)
C1—Sn1—N1—C8	81.5 (4)	C2—C3—C4—C5	−1.9 (13)
S2—Sn1—N1—C8	−44.5 (4)	C3—C4—C5—C6	1.1 (13)
S6—Sn1—N1—C8	−174.9 (4)	C2—C1—C6—C5	0.2 (9)
C10—Sn2—N2—C18	−155.1 (5)	Sn1—C1—C6—C5	178.9 (5)
S1—Sn2—N2—C18	77.0 (5)	C4—C5—C6—C1	−0.2 (11)
S3—Sn2—N2—C18	−49.3 (5)	C9—N1—C7—C2	166.9 (5)
C10—Sn2—N2—C16	−34.5 (4)	C8—N1—C7—C2	−72.5 (6)
S1—Sn2—N2—C16	−162.4 (4)	Sn1—N1—C7—C2	44.5 (5)
S3—Sn2—N2—C16	71.2 (3)	C1—C2—C7—N1	−36.9 (8)
C10—Sn2—N2—C17	81.0 (4)	C3—C2—C7—N1	145.0 (6)
S1—Sn2—N2—C17	−46.9 (4)	S1—Sn2—C10—C15	−87.2 (5)
S3—Sn2—N2—C17	−173.3 (4)	S3—Sn2—C10—C15	114.8 (4)
C19—Sn3—N3—C26	−153.5 (5)	S2—Sn2—C10—C15	12.3 (5)
S5—Sn3—N3—C26	84.4 (4)	N2—Sn2—C10—C15	−161.8 (5)
S3—Sn3—N3—C26	−48.1 (4)	S1—Sn2—C10—C11	94.3 (4)
C19—Sn3—N3—C27	81.0 (4)	S3—Sn2—C10—C11	−63.7 (4)
S5—Sn3—N3—C27	−41.2 (4)	S2—Sn2—C10—C11	−166.2 (4)
S3—Sn3—N3—C27	−173.6 (4)	N2—Sn2—C10—C11	19.7 (4)
C19—Sn3—N3—C25	−34.9 (4)	C15—C10—C11—C12	0.1 (9)
S5—Sn3—N3—C25	−157.1 (3)	Sn2—C10—C11—C12	178.6 (4)
S3—Sn3—N3—C25	70.5 (3)	C15—C10—C11—C16	−179.5 (5)
C28—Sn4—N4—C34	−35.5 (4)	Sn2—C10—C11—C16	−1.0 (7)
S4—Sn4—N4—C34	−161.6 (4)	C10—C11—C12—C13	−0.8 (9)
S6—Sn4—N4—C34	71.0 (4)	C16—C11—C12—C13	178.8 (6)
C28—Sn4—N4—C35	81.2 (5)	C11—C12—C13—C14	1.4 (10)
S4—Sn4—N4—C35	−44.9 (4)	C12—C13—C14—C15	−1.3 (10)
S6—Sn4—N4—C35	−172.3 (4)	C13—C14—C15—C10	0.6 (9)
C28—Sn4—N4—C36	−154.7 (5)	C11—C10—C15—C14	0.0 (8)
S4—Sn4—N4—C36	79.2 (4)	Sn2—C10—C15—C14	−178.4 (4)
S6—Sn4—N4—C36	−48.2 (4)	C18—N2—C16—C11	166.6 (5)
C10—Sn2—S1—Sn1	108.61 (18)	C17—N2—C16—C11	−72.2 (6)
S3—Sn2—S1—Sn1	−98.08 (7)	Sn2—N2—C16—C11	43.6 (5)
S2—Sn2—S1—Sn1	3.71 (6)	C12—C11—C16—N2	146.3 (6)
N2—Sn2—S1—Sn1	176.82 (12)	C10—C11—C16—N2	−34.1 (8)
C1—Sn1—S1—Sn2	−128.22 (16)	S5—Sn3—C19—C20	96.0 (4)
S2—Sn1—S1—Sn2	−3.88 (6)	S3—Sn3—C19—C20	−63.3 (5)
S6—Sn1—S1—Sn2	126.66 (5)	S4—Sn3—C19—C20	−163.7 (4)
C1—Sn1—S2—Sn2	113.3 (2)	N3—Sn3—C19—C20	19.6 (4)
S6—Sn1—S2—Sn2	−99.21 (7)	S5—Sn3—C19—C24	−84.3 (5)
S1—Sn1—S2—Sn2	3.73 (6)	S3—Sn3—C19—C24	116.3 (5)
N1—Sn1—S2—Sn2	−179.89 (12)	S4—Sn3—C19—C24	16.0 (5)
C10—Sn2—S2—Sn1	−130.11 (15)	N3—Sn3—C19—C24	−160.8 (5)
S1—Sn2—S2—Sn1	−3.87 (6)	C24—C19—C20—C21	−0.3 (9)

S3—Sn2—S2—Sn1	122.99 (5)	Sn3—C19—C20—C21	179.4 (5)
C10—Sn2—S3—Sn3	−153.56 (16)	C24—C19—C20—C25	−179.7 (5)
S1—Sn2—S3—Sn3	48.74 (9)	Sn3—C19—C20—C25	−0.1 (7)
S2—Sn2—S3—Sn3	−49.11 (7)	C19—C20—C21—C22	0.2 (10)
N2—Sn2—S3—Sn3	133.43 (13)	C25—C20—C21—C22	179.6 (6)
C19—Sn3—S3—Sn2	−176.05 (17)	C20—C21—C22—C23	0.5 (11)
S5—Sn3—S3—Sn2	28.32 (10)	C21—C22—C23—C24	−1.0 (11)
S4—Sn3—S3—Sn2	−68.48 (7)	C22—C23—C24—C19	0.9 (10)
N3—Sn3—S3—Sn2	110.98 (12)	C20—C19—C24—C23	−0.2 (9)
C28—Sn4—S4—Sn3	113.7 (2)	Sn3—C19—C24—C23	−179.9 (4)
S6—Sn4—S4—Sn3	−98.85 (6)	C26—N3—C25—C20	166.8 (5)
S5—Sn4—S4—Sn3	4.37 (6)	C27—N3—C25—C20	−71.8 (6)
N4—Sn4—S4—Sn3	−179.21 (13)	Sn3—N3—C25—C20	44.6 (5)
C19—Sn3—S4—Sn4	−125.75 (16)	C21—C20—C25—N3	144.4 (6)
S5—Sn3—S4—Sn4	−4.53 (6)	C19—C20—C25—N3	−36.2 (8)
S3—Sn3—S4—Sn4	127.93 (6)	S4—Sn4—C28—C33	−88.6 (5)
C19—Sn3—S5—Sn4	112.83 (18)	S6—Sn4—C28—C33	117.8 (5)
S3—Sn3—S5—Sn4	−94.60 (7)	S5—Sn4—C28—C33	13.5 (5)
S4—Sn3—S5—Sn4	4.35 (6)	N4—Sn4—C28—C33	−161.7 (5)
N3—Sn3—S5—Sn4	−177.57 (12)	S4—Sn4—C28—C29	91.8 (4)
C28—Sn4—S5—Sn3	−129.13 (16)	S6—Sn4—C28—C29	−61.8 (4)
S4—Sn4—S5—Sn3	−4.54 (6)	S5—Sn4—C28—C29	−166.1 (4)
S6—Sn4—S5—Sn3	123.04 (5)	N4—Sn4—C28—C29	18.7 (4)
C1—Sn1—S6—Sn4	−175.42 (17)	C33—C28—C29—C30	0.6 (9)
S2—Sn1—S6—Sn4	32.20 (10)	Sn4—C28—C29—C30	−179.7 (5)
S1—Sn1—S6—Sn4	−67.25 (7)	C33—C28—C29—C34	−178.1 (6)
N1—Sn1—S6—Sn4	112.33 (12)	Sn4—C28—C29—C34	1.5 (7)
C28—Sn4—S6—Sn1	−162.15 (17)	C28—C29—C30—C31	−2.0 (11)
S4—Sn4—S6—Sn1	45.73 (9)	C34—C29—C30—C31	176.7 (7)
S5—Sn4—S6—Sn1	−53.57 (7)	C29—C30—C31—C32	2.1 (13)
N4—Sn4—S6—Sn1	126.13 (14)	C30—C31—C32—C33	−0.8 (13)
S2—Sn1—C1—C2	90.6 (4)	C29—C28—C33—C32	0.6 (9)
S6—Sn1—C1—C2	−64.4 (4)	Sn4—C28—C33—C32	−179.0 (5)
S1—Sn1—C1—C2	−167.4 (4)	C31—C32—C33—C28	−0.5 (11)
N1—Sn1—C1—C2	17.9 (4)	C35—N4—C34—C29	−71.9 (6)
S2—Sn1—C1—C6	−88.2 (5)	C36—N4—C34—C29	166.5 (5)
S6—Sn1—C1—C6	116.8 (5)	Sn4—N4—C34—C29	45.8 (5)
S1—Sn1—C1—C6	13.9 (5)	C30—C29—C34—N4	143.1 (6)
N1—Sn1—C1—C6	−160.9 (5)	C28—C29—C34—N4	−38.2 (8)

Table 1

X—H···π-ring interactions. Cg1 is a centroid of the benzene ring C1–C6, Cg2 is a centroid of the benzene ring C28–C33.

Y—*X*···*Cg*	*X*—H	H···*Cg*	*X*···*Cg*	*X*—H···*Cg*
C30—H30···*Cg*1^{i}	0.93	3.23	3.98 (1)	139
C37—H37···*Cg*2^{ii}	0.98	2.87	3.61 (1)	133

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

Fig. 1

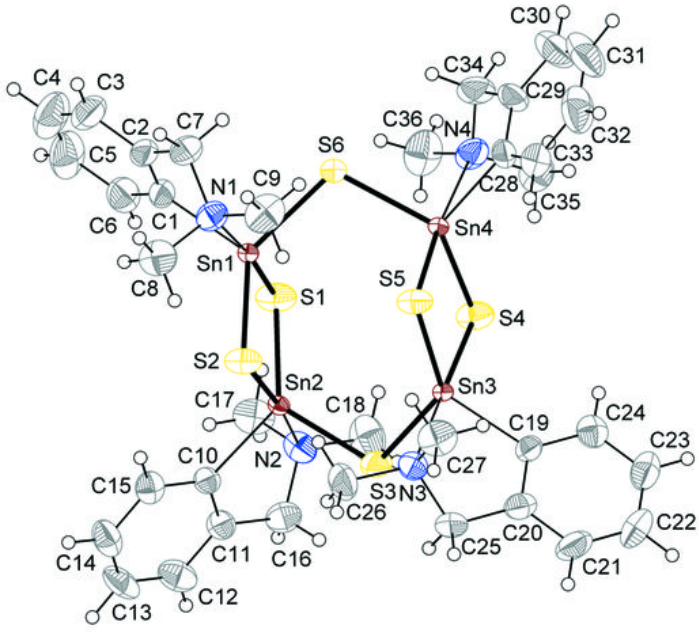
C30
C31
C34
C29
C4
C3
C36
N4
C32
C2
C7
S6
C33
C5
C28
N1
C9
C35
C6
C1
Sn4
Sn1
S5
C8
S1
S4
S2
Sn2
Sn3
C17
C18
C24
C19
C23
C10
N2
C27
C15
S3
N3
C26
C22
C20
C14
C11
C16
C25
C21
C12
C13

Fig. 2

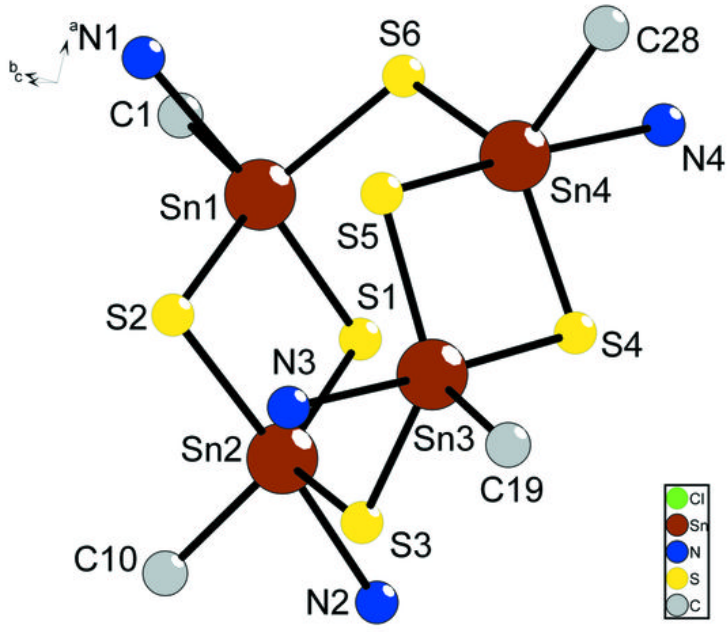
N1
S6
C28
C1
N4
Sn1
Sn4
S5
S1
S2
S4
N3
Sn2
Sn3
C19
S3
C10
N2
Cl
Sn
N
S
C

Fig. 3