

Di-*tert*-butylchlorido(pyrrolidine-1-dithiocarboxylato- κ^2 S,S')tin(IV)

Fahui Li,^{a*} Yantuan Li,^a William T. A. Harrison,^b Weijie Wang^c and Yanping Feng^c

^aMarine Drug and Food Institute, Ocean University of China, Qingdao 266003, People's Republic of China, ^bDepartment of Chemistry, University of Aberdeen, Aberdeen AB24 3UE, Scotland, and ^cCollege of Weifang Science and Technology Vocational, Weifang 262700, People's Republic of China

Correspondence e-mail: liyantuanouc@163.com

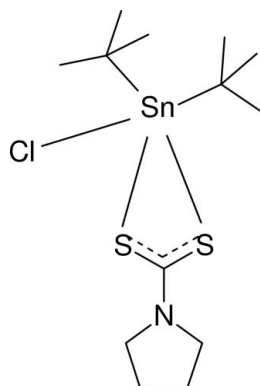
Received 8 November 2007; accepted 29 November 2007

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.010$ Å; disorder in main residue; R factor = 0.044; wR factor = 0.118; data-to-parameter ratio = 27.9.

The title compound, $[\text{Sn}(\text{C}_4\text{H}_9)_2(\text{C}_5\text{H}_8\text{NS}_2)\text{Cl}]$, contains two molecules in the asymmetric unit, with similar conformations. In both molecules, the Sn atom adopts a distorted trigonal-bipyramidal geometry arising from two C atoms, one Cl atom and two S atoms from the bidentate dithiocarbamate ligand, with one Sn—S bond much longer than the other. One C atom of the pyrrolidine ring is disordered equally over two sites.

Related literature

For related structures, see: Ng *et al.* (1989); Furue *et al.* (1970); Hall & Tiekink (1995); Jung & Sohn (1988). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[\text{Sn}(\text{C}_4\text{H}_9)_2(\text{C}_5\text{H}_8\text{NS}_2)\text{Cl}]$	$V = 3741.2$ (13) Å ³
$M_r = 414.61$	$Z = 8$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 12.399$ (3) Å	$\mu = 1.72$ mm ⁻¹
$b = 25.159$ (5) Å	$T = 293$ (2) K
$c = 12.104$ (2) Å	$0.47 \times 0.34 \times 0.29$ mm
$\beta = 97.764$ (3)°	

Data collection

Siemens SMART CCD diffractometer	24292 measured reflections
Absorption correction: multi-scan (SADABS; Siemens, 1996)	9079 independent reflections
$T_{\min} = 0.500$, $T_{\max} = 0.636$	4691 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.048$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$	325 parameters
$wR(F^2) = 0.118$	H-atom parameters constrained
$S = 1.00$	$\Delta\rho_{\text{max}} = 0.99$ e Å ⁻³
9079 reflections	$\Delta\rho_{\text{min}} = -0.46$ e Å ⁻³

Table 1

Selected bond lengths (Å).

Sn1—S1	2.4696 (15)	Sn2—S3	2.4681 (15)
Sn1—S2	2.8264 (16)	Sn2—S4	2.8209 (16)
Sn1—C6	2.190 (6)	Sn2—Cl2	2.4447 (17)
Sn1—C10	2.182 (5)	Sn2—C19	2.187 (6)
Sn1—Cl1	2.4669 (16)	Sn2—C23	2.189 (6)

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

We acknowledge the financial support of the Natural Science Foundation of China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2363).

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Furue, K., Kimura, T., Yasuoka, N., Kasai, N. & Kakudo, M. (1970). *Bull. Chem. Soc. Jpn.*, **43**, 1661–1667.
- Hall, V. J. & Tiekink, E. R. T. (1995). *Main Group Met. Chem.* **18**, 611–620.
- Jung, O. S. & Sohn, Y. S. (1988). *Bull. Kor. Chem. Soc.* **9**, 365–368.
- Ng, S. W., Chen, W., Kumar Das, V. G., Charland, J. P. & Smith, F. E. (1989). *J. Organomet. Chem.* **364**, 343–351.
- Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
- Siemens (1996). *SMART*, *SAINT* and *SADABS*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

supplementary materials

Acta Cryst. (2008). E64, m87 [doi:10.1107/S1600536807064288]

Di-*tert*-butylchlorido(pyrrolidine-1-dithiocarboxylato- κ^2 S,S')tin(IV)

F. Li, Y. Li, W. T. A. Harrison, W. Wang and Y. Feng

Comment

Chlorodialkyltin(IV) derivatives of monobasic chelating ligands generally exist as six-coordinate compounds arising from chloride-ion bridging (Ng *et al.*, 1989). An example of such a compound is chloride-bridged, dimeric chlorodimethyl(*N,N*-dimethyldithiocarbamato)tin, whose crystal structure has been known for a long time (Furue *et al.*, 1970). Replacing the methyl group on tin by the phenyl group interferes with the bridging, as noted in chlorobis(*N*-cyclohexyl-*N*-ethylthiocarbamato)diphenyltin (Hall & Tiekink, 1995).

The sterically bulky *t*-butyl group in the title compound, (I), is also expected to disrupt bridging, and a molecular species results (Fig. 1). There are two molecules in the asymmetric unit, with similar geometries. In both cases, the tin(IV) atom adopts a distorted C₂ClS₂Sn-trigonal bipyramidal geometry (Table 1). The formally double-bonded sulfur atom occupies one of the apical sites and the chloride ion the other in the axially most-electronegative configuration. Otherwise, the geometrical parameters for (I) may be regarded as normal (Allen *et al.*, 1987) and are similar to those found in the other R₂ClSnS₂CNR'₂ mentioned above.

Experimental

The title compound was synthesized by the method described in the literature (Jung & Sohn, 1988). Recrystallization from a 1:1 *v/v* mixture of dichloromethane-hexane yielded colourless blocks of (I). M.P. 439 K. Analysis. Calc. for C₂₆H₅₂N₂S₄ClSn₂: C 37.66, H 6.32; N 3.38%. Found: C 34.43, H 6.18, N 3.52%.

Refinement

Some of the carbon atoms of the *t*-butyl groups show significant anisotropic displacements. Attempts to model this as disorder over two or more sites were not successful. Atom C4 is disordered over two positions in a 0.50 (3):0.50 (3) ratio.

The hydrogen atoms were geometrically placed (C–H = 0.96–0.97 Å), and refined as riding with $U(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$. The methyl groups were allowed to rotate, but not to tip, to best fit the electron density.

Figures

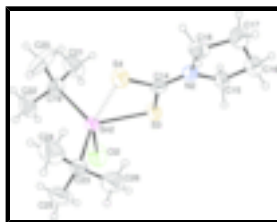


Fig. 1. The molecular structure of the Sn₂ molecule in (I) showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). The long Sn—S contact is shown as a double dashed line.

Di-*tert*-butylchlorido(pyrrolidine-1-dithiocarboxylato- κ^2S,S')tin(IV)

Crystal data

[Sn(C ₄ H ₉) ₂ (C ₅ H ₈ NS ₂)Cl]	$F_{000} = 1680$
$M_r = 414.61$	$D_x = 1.472 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Melting point: 439 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation
$a = 12.399 (3) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 25.159 (5) \text{ \AA}$	Cell parameters from 4903 reflections
$c = 12.104 (2) \text{ \AA}$	$\theta = 2.3\text{--}23.7^\circ$
$\beta = 97.764 (3)^\circ$	$\mu = 1.72 \text{ mm}^{-1}$
$V = 3741.2 (13) \text{ \AA}^3$	$T = 293 (2) \text{ K}$
$Z = 8$	Block, colourless
	$0.47 \times 0.34 \times 0.29 \text{ mm}$

Data collection

Siemens SMART CCD diffractometer	9079 independent reflections
Radiation source: fine-focus sealed tube	4691 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.048$
$T = 293(2) \text{ K}$	$\theta_{\text{max}} = 28.4^\circ$
ω scans	$\theta_{\text{min}} = 1.8^\circ$
Absorption correction: multi-scan (SADABS; Siemens, 1996)	$h = -15 \rightarrow 16$
$T_{\text{min}} = 0.500$, $T_{\text{max}} = 0.636$	$k = -33 \rightarrow 33$
24292 measured reflections	$l = -16 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.118$	$w = 1/[\sigma^2(F_o^2) + (0.0411P)^2 + 2.9577P]$
$S = 1.00$	where $P = (F_o^2 + 2F_c^2)/3$
9079 reflections	$(\Delta/\sigma)_{\text{max}} = 0.002$
325 parameters	$\Delta\rho_{\text{max}} = 0.99 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.46 \text{ e \AA}^{-3}$
	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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Sn1	0.19927 (3)	0.129544 (14)	0.43807 (3)	0.05039 (12)	
C1	0.4091 (4)	0.1000 (2)	0.3436 (4)	0.0530 (13)	
C2	0.5521 (4)	0.0316 (2)	0.3531 (5)	0.0656 (16)	
H2A	0.5050	0.0013	0.3331	0.079*	
H2B	0.5718	0.0323	0.4334	0.079*	
C3	0.6511 (6)	0.0297 (3)	0.2947 (7)	0.122 (3)	
H3A	0.7139	0.0183	0.3459	0.147*	
H3B	0.6402	0.0049	0.2329	0.147*	
C4A	0.6687 (15)	0.0843 (9)	0.253 (2)	0.084 (7)*	0.50 (3)
H4A1	0.7160	0.1044	0.3088	0.101*	0.50 (3)
H4A2	0.7016	0.0830	0.1853	0.101*	0.50 (3)
C4B	0.6406 (14)	0.0636 (8)	0.2067 (18)	0.076 (6)*	0.50 (3)
H4B1	0.6114	0.0450	0.1389	0.091*	0.50 (3)
H4B2	0.7108	0.0784	0.1966	0.091*	0.50 (3)
C5	0.5605 (4)	0.1089 (2)	0.2330 (5)	0.0652 (15)	
H5A	0.5272	0.1031	0.1567	0.078*	
H5B	0.5646	0.1468	0.2476	0.078*	
C6	0.2373 (5)	0.2007 (2)	0.5401 (5)	0.0728 (17)	
C7	0.2331 (6)	0.2489 (3)	0.4688 (7)	0.107 (3)	
H7A	0.1629	0.2513	0.4245	0.161*	
H7B	0.2884	0.2466	0.4206	0.161*	
H7C	0.2452	0.2799	0.5150	0.161*	
C8	0.1499 (8)	0.2060 (3)	0.6171 (7)	0.148 (4)	
H8A	0.1494	0.1746	0.6621	0.222*	
H8B	0.0799	0.2103	0.5731	0.222*	
H8C	0.1653	0.2364	0.6644	0.222*	
C9	0.3471 (7)	0.1940 (3)	0.6056 (8)	0.166 (5)	
H9A	0.3474	0.1629	0.6515	0.249*	
H9B	0.3641	0.2246	0.6520	0.249*	
H9C	0.4004	0.1901	0.5556	0.249*	
C10	0.0631 (5)	0.1179 (3)	0.3061 (5)	0.0694 (17)	
C11	0.0560 (7)	0.1630 (3)	0.2258 (7)	0.138 (4)	
H11A	0.1237	0.1664	0.1962	0.207*	

supplementary materials

H11B	0.0414	0.1953	0.2634	0.207*
H11C	-0.0017	0.1565	0.1661	0.207*
C12	0.0851 (9)	0.0686 (3)	0.2428 (9)	0.189 (6)
H12A	0.1517	0.0729	0.2115	0.284*
H12B	0.0262	0.0627	0.1840	0.284*
H12C	0.0914	0.0387	0.2925	0.284*
C13	-0.0373 (7)	0.1138 (6)	0.3534 (8)	0.251 (8)
H13A	-0.0322	0.0848	0.4055	0.377*
H13B	-0.0964	0.1074	0.2951	0.377*
H13C	-0.0500	0.1462	0.3912	0.377*
N1	0.4993 (3)	0.08164 (16)	0.3120 (4)	0.0540 (11)
S1	0.34854 (12)	0.06438 (6)	0.44053 (13)	0.0652 (4)
S2	0.34882 (13)	0.15709 (6)	0.29081 (14)	0.0707 (4)
Cl1	0.13750 (14)	0.07141 (7)	0.58121 (14)	0.0856 (5)
Sn2	0.76534 (3)	0.139079 (15)	0.85114 (3)	0.05640 (13)
C14	0.7473 (4)	0.0294 (2)	0.9603 (4)	0.0560 (14)
C15	0.8512 (5)	-0.0358 (2)	1.0835 (5)	0.0699 (16)
H15A	0.8583	-0.0177	1.1548	0.084*
H15B	0.9170	-0.0303	1.0498	0.084*
C16	0.8299 (6)	-0.0941 (3)	1.0971 (7)	0.098 (2)
H16A	0.8627	-0.1148	1.0429	0.117*
H16B	0.8592	-0.1060	1.1713	0.117*
C17	0.7135 (6)	-0.0995 (3)	1.0794 (7)	0.109 (3)
H17A	0.6839	-0.0942	1.1487	0.130*
H17B	0.6933	-0.1348	1.0516	0.130*
C18	0.6694 (5)	-0.0577 (2)	0.9943 (5)	0.0731 (17)
H18A	0.6606	-0.0719	0.9191	0.088*
H18B	0.6002	-0.0437	1.0101	0.088*
C19	0.6519 (5)	0.1953 (2)	0.9113 (5)	0.0738 (17)
C20	0.5356 (6)	0.1769 (4)	0.8820 (9)	0.170 (5)
H20A	0.5186	0.1739	0.8025	0.255*
H20B	0.4876	0.2023	0.9092	0.255*
H20C	0.5267	0.1429	0.9157	0.255*
C21	0.6793 (8)	0.1989 (3)	1.0358 (6)	0.128 (3)
H21A	0.7530	0.2110	1.0544	0.192*
H21B	0.6718	0.1644	1.0681	0.192*
H21C	0.6308	0.2234	1.0645	0.192*
C22	0.6713 (8)	0.2495 (3)	0.8622 (7)	0.133 (3)
H22A	0.6560	0.2478	0.7824	0.199*
H22B	0.7458	0.2597	0.8835	0.199*
H22C	0.6242	0.2752	0.8897	0.199*
C23	0.7730 (6)	0.1232 (3)	0.6746 (5)	0.0767 (18)
C24	0.6554 (7)	0.1218 (4)	0.6157 (6)	0.129 (3)
H24A	0.6163	0.0939	0.6468	0.194*
H24B	0.6556	0.1155	0.5375	0.194*
H24C	0.6208	0.1553	0.6258	0.194*
C25	0.8356 (7)	0.1679 (3)	0.6291 (7)	0.130 (3)
H25A	0.7991	0.2010	0.6377	0.194*
H25B	0.8397	0.1618	0.5515	0.194*

H25C	0.9078	0.1694	0.6693	0.194*
C26	0.8287 (8)	0.0714 (3)	0.6631 (7)	0.140 (4)
H26A	0.7891	0.0436	0.6940	0.210*
H26B	0.9013	0.0730	0.7021	0.210*
H26C	0.8315	0.0643	0.5856	0.210*
N2	0.7552 (3)	-0.01685 (17)	1.0098 (4)	0.0564 (11)
S3	0.85602 (11)	0.07357 (6)	0.98437 (14)	0.0682 (4)
S4	0.63452 (12)	0.04916 (7)	0.87493 (14)	0.0756 (5)
Cl2	0.92997 (15)	0.19225 (7)	0.89949 (19)	0.1153 (8)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0460 (2)	0.0545 (2)	0.0514 (2)	0.00284 (17)	0.00948 (16)	0.00291 (18)
C1	0.045 (3)	0.055 (3)	0.062 (4)	-0.001 (2)	0.017 (3)	-0.005 (3)
C2	0.061 (4)	0.067 (4)	0.070 (4)	0.017 (3)	0.013 (3)	0.005 (3)
C3	0.099 (6)	0.154 (8)	0.127 (7)	0.070 (6)	0.065 (5)	0.029 (6)
C5	0.063 (4)	0.075 (4)	0.062 (4)	0.003 (3)	0.025 (3)	0.002 (3)
C6	0.083 (5)	0.059 (4)	0.075 (4)	0.004 (3)	0.007 (4)	-0.014 (3)
C7	0.124 (7)	0.066 (4)	0.131 (7)	-0.003 (4)	0.016 (5)	-0.013 (5)
C8	0.219 (11)	0.107 (6)	0.140 (8)	-0.004 (7)	0.104 (8)	-0.043 (6)
C9	0.147 (8)	0.129 (7)	0.192 (10)	0.018 (6)	-0.091 (8)	-0.068 (7)
C10	0.059 (4)	0.081 (4)	0.065 (4)	-0.011 (3)	-0.006 (3)	0.007 (3)
C11	0.130 (7)	0.132 (7)	0.132 (7)	-0.007 (6)	-0.056 (6)	0.028 (6)
C12	0.200 (11)	0.130 (7)	0.198 (11)	0.039 (7)	-0.118 (9)	-0.075 (8)
C13	0.050 (5)	0.57 (3)	0.123 (8)	-0.049 (10)	-0.010 (5)	0.051 (12)
N1	0.050 (3)	0.058 (3)	0.056 (3)	0.007 (2)	0.016 (2)	0.001 (2)
S1	0.0643 (10)	0.0593 (9)	0.0771 (11)	0.0141 (7)	0.0283 (8)	0.0201 (8)
S2	0.0653 (10)	0.0629 (9)	0.0900 (12)	0.0163 (7)	0.0326 (9)	0.0275 (8)
Cl1	0.0828 (12)	0.0949 (12)	0.0859 (12)	0.0063 (9)	0.0361 (9)	0.0295 (10)
Sn2	0.0486 (2)	0.0586 (2)	0.0612 (3)	-0.00115 (17)	0.00451 (18)	0.00429 (19)
C14	0.048 (3)	0.068 (4)	0.052 (3)	-0.002 (3)	0.009 (3)	0.000 (3)
C15	0.068 (4)	0.064 (4)	0.078 (4)	0.003 (3)	0.011 (3)	0.012 (3)
C16	0.105 (6)	0.075 (5)	0.116 (6)	0.009 (4)	0.024 (5)	0.023 (4)
C17	0.105 (6)	0.055 (4)	0.171 (8)	-0.008 (4)	0.040 (6)	0.014 (5)
C18	0.067 (4)	0.066 (4)	0.089 (5)	-0.024 (3)	0.017 (3)	-0.009 (4)
C19	0.083 (5)	0.068 (4)	0.072 (5)	0.013 (3)	0.016 (3)	-0.008 (3)
C20	0.073 (6)	0.157 (9)	0.279 (14)	0.034 (6)	0.022 (7)	-0.076 (9)
C21	0.226 (10)	0.084 (5)	0.081 (6)	0.014 (6)	0.049 (6)	-0.005 (4)
C22	0.204 (10)	0.085 (5)	0.115 (7)	0.061 (6)	0.046 (6)	0.025 (5)
C23	0.092 (5)	0.075 (4)	0.068 (4)	0.005 (4)	0.029 (4)	0.003 (3)
C24	0.147 (8)	0.175 (8)	0.061 (5)	-0.006 (7)	-0.002 (5)	-0.008 (5)
C25	0.174 (9)	0.121 (7)	0.109 (7)	-0.010 (6)	0.077 (6)	0.022 (5)
C26	0.212 (10)	0.089 (6)	0.138 (8)	0.040 (6)	0.092 (7)	-0.001 (5)
N2	0.053 (3)	0.057 (3)	0.060 (3)	-0.003 (2)	0.009 (2)	0.002 (2)
S3	0.0478 (8)	0.0676 (9)	0.0841 (11)	-0.0126 (7)	-0.0103 (8)	0.0192 (8)
S4	0.0508 (9)	0.0848 (11)	0.0855 (12)	-0.0142 (8)	-0.0108 (8)	0.0149 (9)
Cl2	0.0780 (12)	0.0915 (12)	0.167 (2)	-0.0381 (10)	-0.0170 (12)	0.0282 (13)

supplementary materials

Geometric parameters (Å, °)

Sn1—S1	2.4696 (15)	C13—H13B	0.9600
Sn1—S2	2.8264 (16)	C13—H13C	0.9600
Sn1—C6	2.190 (6)	Sn2—S3	2.4681 (15)
Sn1—C10	2.182 (5)	Sn2—S4	2.8209 (16)
Sn1—C11	2.4669 (16)	Sn2—C12	2.4447 (17)
C1—N1	1.313 (6)	Sn2—C19	2.187 (6)
C1—S2	1.704 (5)	Sn2—C23	2.189 (6)
C1—S1	1.726 (5)	C14—N2	1.306 (6)
C2—N1	1.475 (6)	C14—S4	1.697 (5)
C2—C3	1.498 (8)	C14—S3	1.741 (5)
C2—H2A	0.9700	C15—N2	1.468 (7)
C2—H2B	0.9700	C15—C16	1.502 (8)
C3—C4B	1.357 (14)	C15—H15A	0.9700
C3—C4A	1.487 (18)	C15—H15B	0.9700
C3—H3A	0.9700	C16—C17	1.437 (9)
C3—H3B	0.9700	C16—H16A	0.9700
C4A—C5	1.467 (14)	C16—H16B	0.9700
C4A—H4A1	0.9700	C17—C18	1.521 (9)
C4A—H4A2	0.9700	C17—H17A	0.9700
C4B—C5	1.573 (16)	C17—H17B	0.9700
C4B—H4B1	0.9700	C18—N2	1.473 (6)
C4B—H4B2	0.9700	C18—H18A	0.9700
C5—N1	1.469 (6)	C18—H18B	0.9700
C5—H5A	0.9700	C19—C21	1.502 (9)
C5—H5B	0.9700	C19—C20	1.510 (10)
C6—C7	1.484 (8)	C19—C22	1.520 (9)
C6—C9	1.490 (9)	C20—H20A	0.9600
C6—C8	1.528 (9)	C20—H20B	0.9600
C7—H7A	0.9600	C20—H20C	0.9600
C7—H7B	0.9600	C21—H21A	0.9600
C7—H7C	0.9600	C21—H21B	0.9600
C8—H8A	0.9600	C21—H21C	0.9600
C8—H8B	0.9600	C22—H22A	0.9600
C8—H8C	0.9600	C22—H22B	0.9600
C9—H9A	0.9600	C22—H22C	0.9600
C9—H9B	0.9600	C23—C26	1.490 (9)
C9—H9C	0.9600	C23—C25	1.512 (9)
C10—C13	1.443 (10)	C23—C24	1.534 (10)
C10—C11	1.489 (9)	C24—H24A	0.9600
C10—C12	1.502 (10)	C24—H24B	0.9600
C11—H11A	0.9600	C24—H24C	0.9600
C11—H11B	0.9600	C25—H25A	0.9600
C11—H11C	0.9600	C25—H25B	0.9600
C12—H12A	0.9600	C25—H25C	0.9600
C12—H12B	0.9600	C26—H26A	0.9600
C12—H12C	0.9600	C26—H26B	0.9600

C13—H13A	0.9600	C26—H26C	0.9600
C10—Sn1—C6	127.5 (2)	H13A—C13—H13C	109.5
C10—Sn1—Cl1	98.75 (17)	H13B—C13—H13C	109.5
C6—Sn1—Cl1	98.76 (18)	C1—N1—C5	124.1 (4)
C10—Sn1—S1	115.12 (18)	C1—N1—C2	123.9 (4)
C6—Sn1—S1	115.61 (17)	C5—N1—C2	112.0 (4)
Cl1—Sn1—S1	84.33 (5)	C1—S1—Sn1	92.39 (18)
C10—Sn1—S2	94.56 (17)	C1—S2—Sn1	81.30 (18)
C6—Sn1—S2	92.62 (18)	C19—Sn2—C23	123.9 (2)
Cl1—Sn1—S2	151.72 (5)	C19—Sn2—Cl2	96.91 (18)
S1—Sn1—S2	67.41 (5)	C23—Sn2—Cl2	100.86 (19)
N1—C1—S2	122.3 (4)	C19—Sn2—S3	118.09 (18)
N1—C1—S1	118.8 (4)	C23—Sn2—S3	116.12 (18)
S2—C1—S1	118.9 (3)	Cl2—Sn2—S3	85.24 (6)
N1—C2—C3	102.8 (5)	C19—Sn2—S4	94.58 (18)
N1—C2—H2A	111.2	C23—Sn2—S4	93.15 (18)
C3—C2—H2A	111.2	Cl2—Sn2—S4	152.55 (6)
N1—C2—H2B	111.2	S3—Sn2—S4	67.37 (5)
C3—C2—H2B	111.2	N2—C14—S4	123.0 (4)
H2A—C2—H2B	109.1	N2—C14—S3	118.9 (4)
C4B—C3—C4A	32.8 (7)	S4—C14—S3	118.1 (3)
C4B—C3—C2	110.7 (8)	N2—C15—C16	104.1 (5)
C4A—C3—C2	107.2 (8)	N2—C15—H15A	110.9
C4B—C3—H3A	132.1	C16—C15—H15A	110.9
C4A—C3—H3A	110.3	N2—C15—H15B	110.9
C2—C3—H3A	110.3	C16—C15—H15B	110.9
C4B—C3—H3B	79.0	H15A—C15—H15B	108.9
C4A—C3—H3B	110.3	C17—C16—C15	105.4 (6)
C2—C3—H3B	110.3	C17—C16—H16A	110.7
H3A—C3—H3B	108.5	C15—C16—H16A	110.7
C5—C4A—C3	105.9 (12)	C17—C16—H16B	110.7
C5—C4A—H4A1	110.6	C15—C16—H16B	110.7
C3—C4A—H4A1	110.6	H16A—C16—H16B	108.8
C5—C4A—H4A2	110.6	C16—C17—C18	107.3 (6)
C3—C4A—H4A2	110.6	C16—C17—H17A	110.3
H4A1—C4A—H4A2	108.7	C18—C17—H17A	110.3
C3—C4B—C5	107.0 (11)	C16—C17—H17B	110.3
C3—C4B—H4B1	110.3	C18—C17—H17B	110.3
C5—C4B—H4B1	110.3	H17A—C17—H17B	108.5
C3—C4B—H4B2	110.3	N2—C18—C17	102.1 (5)
C5—C4B—H4B2	110.3	N2—C18—H18A	111.4
H4B1—C4B—H4B2	108.6	C17—C18—H18A	111.3
C4A—C5—N1	103.5 (7)	N2—C18—H18B	111.3
C4A—C5—C4B	30.8 (7)	C17—C18—H18B	111.3
N1—C5—C4B	100.9 (6)	H18A—C18—H18B	109.2
C4A—C5—H5A	111.1	C21—C19—C20	109.5 (7)
N1—C5—H5A	111.1	C21—C19—C22	108.2 (6)
C4B—C5—H5A	84.1	C20—C19—C22	112.3 (7)
C4A—C5—H5B	111.1	C21—C19—Sn2	107.7 (5)

supplementary materials

N1—C5—H5B	111.1	C20—C19—Sn2	111.2 (5)
C4B—C5—H5B	137.0	C22—C19—Sn2	107.9 (5)
H5A—C5—H5B	109.0	C19—C20—H20A	109.5
C7—C6—C9	111.1 (7)	C19—C20—H20B	109.5
C7—C6—C8	108.2 (6)	H20A—C20—H20B	109.5
C9—C6—C8	110.9 (7)	C19—C20—H20C	109.5
C7—C6—Sn1	110.6 (4)	H20A—C20—H20C	109.5
C9—C6—Sn1	108.6 (4)	H20B—C20—H20C	109.5
C8—C6—Sn1	107.4 (5)	C19—C21—H21A	109.5
C6—C7—H7A	109.5	C19—C21—H21B	109.5
C6—C7—H7B	109.5	H21A—C21—H21B	109.5
H7A—C7—H7B	109.5	C19—C21—H21C	109.5
C6—C7—H7C	109.5	H21A—C21—H21C	109.5
H7A—C7—H7C	109.5	H21B—C21—H21C	109.5
H7B—C7—H7C	109.5	C19—C22—H22A	109.5
C6—C8—H8A	109.5	C19—C22—H22B	109.5
C6—C8—H8B	109.5	H22A—C22—H22B	109.5
H8A—C8—H8B	109.5	C19—C22—H22C	109.5
C6—C8—H8C	109.5	H22A—C22—H22C	109.5
H8A—C8—H8C	109.5	H22B—C22—H22C	109.5
H8B—C8—H8C	109.5	C26—C23—C25	110.5 (6)
C6—C9—H9A	109.5	C26—C23—C24	111.1 (7)
C6—C9—H9B	109.5	C25—C23—C24	110.5 (6)
H9A—C9—H9B	109.5	C26—C23—Sn2	109.4 (5)
C6—C9—H9C	109.5	C25—C23—Sn2	108.2 (5)
H9A—C9—H9C	109.5	C24—C23—Sn2	107.1 (4)
H9B—C9—H9C	109.5	C23—C24—H24A	109.5
C13—C10—C11	109.7 (8)	C23—C24—H24B	109.5
C13—C10—C12	111.6 (8)	H24A—C24—H24B	109.5
C11—C10—C12	107.2 (7)	C23—C24—H24C	109.5
C13—C10—Sn1	110.0 (5)	H24A—C24—H24C	109.5
C11—C10—Sn1	110.3 (4)	H24B—C24—H24C	109.5
C12—C10—Sn1	107.9 (4)	C23—C25—H25A	109.5
C10—C11—H11A	109.5	C23—C25—H25B	109.5
C10—C11—H11B	109.5	H25A—C25—H25B	109.5
H11A—C11—H11B	109.5	C23—C25—H25C	109.5
C10—C11—H11C	109.5	H25A—C25—H25C	109.5
H11A—C11—H11C	109.5	H25B—C25—H25C	109.5
H11B—C11—H11C	109.5	C23—C26—H26A	109.5
C10—C12—H12A	109.5	C23—C26—H26B	109.5
C10—C12—H12B	109.5	H26A—C26—H26B	109.5
H12A—C12—H12B	109.5	C23—C26—H26C	109.5
C10—C12—H12C	109.5	H26A—C26—H26C	109.5
H12A—C12—H12C	109.5	H26B—C26—H26C	109.5
H12B—C12—H12C	109.5	C14—N2—C15	125.0 (4)
C10—C13—H13A	109.5	C14—N2—C18	123.7 (5)
C10—C13—H13B	109.5	C15—N2—C18	111.3 (4)
H13A—C13—H13B	109.5	C14—S3—Sn2	92.45 (19)
C10—C13—H13C	109.5	C14—S4—Sn2	81.93 (19)

N1—C2—C3—C4B	-17.3 (14)	C10—Sn1—S2—C1	-115.9 (2)
N1—C2—C3—C4A	17.2 (13)	C6—Sn1—S2—C1	116.2 (2)
C4B—C3—C4A—C5	72.6 (19)	Cl1—Sn1—S2—C1	2.2 (2)
C2—C3—C4A—C5	-29.0 (19)	S1—Sn1—S2—C1	-0.57 (18)
C4A—C3—C4B—C5	-63.5 (17)	N2—C15—C16—C17	-26.0 (8)
C2—C3—C4B—C5	26.4 (19)	C15—C16—C17—C18	32.6 (8)
C3—C4A—C5—N1	28.0 (18)	C16—C17—C18—N2	-25.7 (7)
C3—C4A—C5—C4B	-60.7 (17)	C23—Sn2—C19—C21	-174.5 (5)
C3—C4B—C5—C4A	74.0 (19)	Cl2—Sn2—C19—C21	-66.4 (5)
C3—C4B—C5—N1	-24.2 (17)	S3—Sn2—C19—C21	21.9 (5)
C10—Sn1—C6—C7	-48.4 (6)	S4—Sn2—C19—C21	88.6 (5)
Cl1—Sn1—C6—C7	-156.6 (5)	C23—Sn2—C19—C20	65.6 (7)
S1—Sn1—C6—C7	115.6 (5)	Cl2—Sn2—C19—C20	173.7 (6)
S2—Sn1—C6—C7	49.4 (5)	S3—Sn2—C19—C20	-98.1 (6)
C10—Sn1—C6—C9	-170.5 (6)	S4—Sn2—C19—C20	-31.3 (6)
Cl1—Sn1—C6—C9	81.3 (6)	C23—Sn2—C19—C22	-57.9 (6)
S1—Sn1—C6—C9	-6.6 (6)	Cl2—Sn2—C19—C22	50.1 (5)
S2—Sn1—C6—C9	-72.7 (6)	S3—Sn2—C19—C22	138.4 (4)
C10—Sn1—C6—C8	69.4 (6)	S4—Sn2—C19—C22	-154.8 (5)
Cl1—Sn1—C6—C8	-38.7 (5)	C19—Sn2—C23—C26	-160.5 (5)
S1—Sn1—C6—C8	-126.6 (5)	Cl2—Sn2—C23—C26	93.5 (5)
S2—Sn1—C6—C8	167.2 (5)	S3—Sn2—C23—C26	3.5 (6)
C6—Sn1—C10—C13	-71.1 (8)	S4—Sn2—C23—C26	-62.8 (5)
Cl1—Sn1—C10—C13	37.1 (8)	C19—Sn2—C23—C25	79.1 (6)
S1—Sn1—C10—C13	124.9 (8)	Cl2—Sn2—C23—C25	-26.9 (5)
S2—Sn1—C10—C13	-167.9 (8)	S3—Sn2—C23—C25	-116.9 (5)
C6—Sn1—C10—C11	50.0 (6)	S4—Sn2—C23—C25	176.8 (5)
Cl1—Sn1—C10—C11	158.2 (5)	C19—Sn2—C23—C24	-40.0 (6)
S1—Sn1—C10—C11	-113.9 (5)	Cl2—Sn2—C23—C24	-146.0 (5)
S2—Sn1—C10—C11	-46.8 (5)	S3—Sn2—C23—C24	124.0 (4)
C6—Sn1—C10—C12	166.9 (6)	S4—Sn2—C23—C24	57.7 (5)
Cl1—Sn1—C10—C12	-84.9 (6)	S4—C14—N2—C15	179.5 (4)
S1—Sn1—C10—C12	2.9 (6)	S3—C14—N2—C15	-1.7 (8)
S2—Sn1—C10—C12	70.1 (6)	S4—C14—N2—C18	2.3 (8)
S2—C1—N1—C5	2.9 (7)	S3—C14—N2—C18	-178.9 (4)
S1—C1—N1—C5	-178.0 (4)	C16—C15—N2—C14	-167.6 (5)
S2—C1—N1—C2	-178.1 (4)	C16—C15—N2—C18	10.0 (7)
S1—C1—N1—C2	1.0 (7)	C17—C18—N2—C14	-173.5 (6)
C4A—C5—N1—C1	161.3 (13)	C17—C18—N2—C15	8.9 (6)
C4B—C5—N1—C1	-167.3 (11)	N2—C14—S3—Sn2	176.6 (4)
C4A—C5—N1—C2	-17.8 (13)	S4—C14—S3—Sn2	-4.5 (3)
C4B—C5—N1—C2	13.6 (11)	C19—Sn2—S3—C14	85.4 (3)
C3—C2—N1—C1	-178.7 (6)	C23—Sn2—S3—C14	-79.5 (3)
C3—C2—N1—C5	0.4 (7)	Cl2—Sn2—S3—C14	-179.3 (2)
N1—C1—S1—Sn1	179.9 (4)	S4—Sn2—S3—C14	2.58 (18)
S2—C1—S1—Sn1	-1.0 (3)	N2—C14—S4—Sn2	-177.2 (5)
C10—Sn1—S1—C1	84.8 (3)	S3—C14—S4—Sn2	4.0 (3)
C6—Sn1—S1—C1	-81.1 (3)	C19—Sn2—S4—C14	-121.3 (3)
Cl1—Sn1—S1—C1	-178.15 (18)	C23—Sn2—S4—C14	114.4 (3)

supplementary materials

S2—Sn1—S1—C1	0.56 (18)	Cl2—Sn2—S4—C14	-6.7 (3)
N1—C1—S2—Sn1	179.9 (5)	S3—Sn2—S4—C14	-2.67 (19)
S1—C1—S2—Sn1	0.9 (3)		

Fig. 1

