Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(4-Amino-3-phenyl-5-thioxo-4,5-dihydro-1*H*-1,2,4-triazol-1-yl)triphenyltin(IV)

Qingfeng Wang, Rufen Zhang* and Lingyun Du

Department of Chemistry, Liaocheng University, Liaocheng 252059, People's Republic of China
Correspondence e-mail: macl@lcu.edu.cn

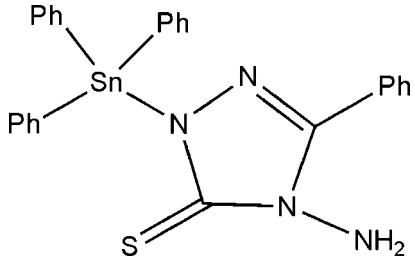
Received 29 October 2007; accepted 2 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.012 Å; R factor = 0.051; wR factor = 0.122; data-to-parameter ratio = 14.1.

In the title complex, $[Sn(C_6H_5)_3(C_8H_7N_4S)]$, all bond lengths and angles show normal values. The Sn centre is four-coordinated by three C atoms [Sn—C 2.119 (6)–2.133 (6) Å] and one N atom [Sn—N 2.107 (5) Å] in a distorted tetrahedral geometry. The crystal packing exhibits no classical intermolecular hydrogen bonds.

Related literature

For related literature, see: Dubey & Roy (2003); Gielen (2002); Li *et al.* (2005).



Experimental

Crystal data

$[Sn(C_6H_5)_3(C_8H_7N_4S)]$
M_r = 541.23
Triclinic, $P\overline{1}$
a = 8.964 (8) Å
b = 9.656 (8) Å
c = 15.481 (13) Å
α = 84.423 (10)°
β = 86.911 (10)°
γ = 63.110 (8)°
V = 1189.4 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 293 (2) K
0.60 × 0.54 × 0.48 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.537, T_{max} = 0.601
(expected range = 0.507–0.567)
5879 measured reflections
4066 independent reflections
2892 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.122
S = 1.00
4066 reflections
289 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.92 e Å^{-3}

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

The authors thank the National Natural Science Foundation of China (grant No. 20271025) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2338).

References

Dubey, S. K. & Roy, U. (2003). *Appl. Organomet. Chem.* **17**, 3–8.
Gielen, M. (2002). *Appl. Organomet. Chem.* **16**, 481–494.
Li, Y.-X., Zhang, R.-F. & Ma, C.-L. (2005). *Acta Cryst.* E**61**, m2365–m2366.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

 doi:10.1107/S1600536807055560

supplementary materials

Acta Cryst. (2007). E**63**, m2959 [**doi:10.1107/S1600536807055560**]

(4-Amino-3-phenyl-5-thioxo-4,5-dihydro-1*H*-1,2,4-triazol-1-yl)triphenyltin(IV)

Q. Wang, R. Zhang and L. Du

Comment

In recent years, organotin complexes have been attracting more and more attention for their wide industrial applications and biological activities (Dubey & Roy, 2003). In order to explore the relationships between the properties and structures, a large number of organotin complexes have been prepared (Gielen, 2002). We report here the structure of the title mononuclear Sn(IV) complex, (I).

The molecular structure of complex (I) is shown in Fig. 1. Sn1 is four-coordinated in a distorted tetrahedron geometry. The Sn—N bond distance is comparable to that found in [phenyl-tris(pyrimidine-2-thiolato)tin(IV)] (Li *et al.*, 2005). The bond angles at the Sn1 atom range from 99.9 (2) to 110.7 (2)°. The crystal packing exhibits no classical intermolecular hydrogen bonds.

Experimental

The reaction was carried out under nitrogen atmoshpere. 4-Amino-5-phenyl-4*H*-1,2,4-triazole-3-thiol (0.192 g, 1 mmol) was added to the solution of benzene (30 ml) with sodium ethoxide (0.68 g, 1 mmol) in a Schlenk flask. After stirring for 10 min, triphenyltin chloride (0.385 g, 1 mmol) was added to the mixture. The mixture was kept at 313 K for 12 h. After cooling down to the room temperature, the solution was filtered. The solvent of the filtrate was gradually removed by evaporation under vacuum until a solid product was obtained. The solid was then recrystallized from diethyl ether. Colourless single crystals of the title complex were obtained after one week. Yield, 87%. Analysis calculated for $C_{26}H_{22}N_4S_1Sn_1$: C 57.70, H 4.10, N, 10.35; found: C 57.91, H 4.29, N, 10.09. The elemental analyses were performed with PERKIN ELMER MODEL 2400 SERIES II.

Refinement

All H atoms were placed in geometrically idealized positions (C—H = 0.93 Å and N—H = 0.86 Å) and treated as riding on their parent atoms, with U_{iso}(H) = 1.2U_{eq} of the parent atom.

Figures

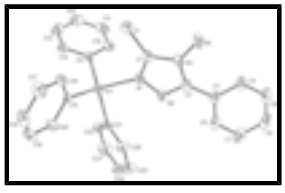


Fig. 1. The molecular structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms omitted for clarity.

Triphenyl(4-amino-5-phenyl-4*H*-1,2,4-triazole-3-thiol-κN^2)tin(IV)

Crystal data

$[Sn(C_6H_5)_3(C_8H_7N_4S)]$	$Z = 2$
$M_r = 541.23$	$F_{000} = 544$
Triclinic, $P\overline{1}$	$D_x = 1.511$ Mg m^{-3}
Hall symbol: -P1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.964$ (8) Å	Cell parameters from 2210 reflections
$b = 9.656$ (8) Å	$\theta = 2.4$–23.8º
$c = 15.481$ (13) Å	$\mu = 1.18$ mm^{-1}
$\alpha = 84.423$ (10)º	$T = 293$ (2) K
$\beta = 86.911$ (10)º	Block, colourless
$\gamma = 63.110$ (8)º	0.60 × 0.54 × 0.48 mm
$V = 1189.4$ (18) Å^3	

Data collection

Siemens SMART CCD area-detector diffractometer	4066 independent reflections
Radiation source: fine-focus sealed tube	2892 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.043$
$T = 293(2)$ K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 2.4$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -7 \rightarrow 10$
$T_{min} = 0.537$, $T_{max} = 0.601$	$k = -11 \rightarrow 11$
5879 measured reflections	$l = -18 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H-atom parameters constrained
$wR(F^2) = 0.122$	$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
4066 reflections	$\Delta\rho_{max} = 1.09$ e Å^{-3}
289 parameters	$\Delta\rho_{min} = -0.92$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.23422 (6)	0.73462 (6)	0.79295 (3)	0.03700 (19)
N1	0.1773 (7)	0.6966 (6)	0.6698 (3)	0.0366 (13)
N2	0.2770 (7)	0.5565 (6)	0.6339 (3)	0.0416 (14)
N3	0.0812 (7)	0.7134 (6)	0.5445 (3)	0.0364 (13)
N4	−0.0199 (8)	0.7765 (7)	0.4711 (3)	0.0560 (18)
H4A	−0.0001	0.7230	0.4269	0.067*
H4B	−0.1018	0.8687	0.4702	0.067*
S1	−0.0960 (2)	0.9684 (2)	0.63727 (13)	0.0499 (5)
C1	0.0562 (8)	0.7946 (8)	0.6174 (4)	0.0348 (16)
C2	0.2143 (8)	0.5715 (8)	0.5573 (4)	0.0375 (16)
C3	0.2865 (9)	0.4439 (8)	0.4994 (4)	0.0416 (17)
C4	0.2067 (10)	0.4278 (9)	0.4301 (4)	0.053 (2)
H4	0.1001	0.5052	0.4158	0.063*
C5	0.2786 (12)	0.3024 (11)	0.3821 (5)	0.061 (2)
H5	0.2230	0.2981	0.3342	0.073*
C6	0.4307 (13)	0.1835 (10)	0.4034 (6)	0.070 (3)
H6	0.4776	0.0956	0.3722	0.084*
C7	0.5135 (12)	0.1961 (10)	0.4718 (6)	0.073 (3)
H7	0.6190	0.1173	0.4867	0.088*
C8	0.4400 (11)	0.3256 (9)	0.5185 (5)	0.060 (2)
H8	0.4978	0.3321	0.5648	0.072*
C9	0.0375 (8)	0.7371 (7)	0.8760 (4)	0.0331 (15)
C10	−0.0341 (9)	0.6419 (9)	0.8663 (5)	0.053 (2)
H10	−0.0005	0.5783	0.8205	0.064*
C11	−0.1562 (9)	0.6389 (10)	0.9236 (6)	0.066 (2)
H11	−0.2037	0.5730	0.9163	0.079*
C12	−0.2080 (10)	0.7327 (11)	0.9915 (6)	0.068 (2)
H12	−0.2900	0.7304	1.0303	0.082*
C13	−0.1382 (11)	0.8281 (11)	1.0009 (5)	0.070 (3)
H13	−0.1730	0.8925	1.0463	0.084*
C14	−0.0169 (9)	0.8311 (8)	0.9445 (4)	0.0459 (18)
H14	0.0299	0.8974	0.9523	0.055*
C15	0.2901 (7)	0.9268 (7)	0.7841 (4)	0.0302 (15)

C16	0.1941 (9)	1.0706 (8)	0.7417 (5)	0.0481 (19)
H16	0.0926	1.0906	0.7178	0.058*
C17	0.2463 (10)	1.1841 (9)	0.7344 (5)	0.061 (2)
H17	0.1796	1.2803	0.7056	0.073*
C18	0.3940 (11)	1.1589 (10)	0.7684 (5)	0.064 (2)
H18	0.4290	1.2365	0.7629	0.077*
C19	0.4886 (10)	1.0189 (11)	0.8105 (6)	0.064 (2)
H19	0.5893	1.0007	0.8345	0.077*
C20	0.4395 (8)	0.9031 (9)	0.8184 (5)	0.0486 (19)
H20	0.5075	0.8074	0.8473	0.058*
C21	0.4577 (8)	0.5244 (7)	0.8192 (4)	0.0346 (16)
C22	0.4786 (9)	0.4393 (9)	0.8978 (5)	0.0482 (19)
H22	0.3958	0.4741	0.9404	0.058*
C23	0.6228 (11)	0.3018 (10)	0.9135 (6)	0.071 (3)
H23	0.6360	0.2426	0.9662	0.085*
C24	0.7458 (10)	0.2530 (11)	0.8516 (7)	0.075 (3)
H24	0.8437	0.1615	0.8626	0.089*
C25	0.7260 (10)	0.3372 (10)	0.7739 (6)	0.068 (2)
H25	0.8097	0.3024	0.7317	0.081*
C26	0.5835 (8)	0.4730 (9)	0.7575 (5)	0.051 (2)
H26	0.5714	0.5310	0.7044	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0371 (3)	0.0410 (3)	0.0347 (3)	−0.0189 (2)	0.0001 (2)	−0.0043 (2)
N1	0.042 (3)	0.041 (4)	0.027 (3)	−0.019 (3)	−0.002 (3)	−0.006 (3)
N2	0.048 (4)	0.037 (4)	0.035 (3)	−0.015 (3)	−0.006 (3)	0.000 (3)
N3	0.045 (4)	0.040 (4)	0.027 (3)	−0.022 (3)	−0.009 (3)	0.004 (3)
N4	0.080 (5)	0.050 (4)	0.032 (3)	−0.022 (4)	−0.020 (3)	−0.002 (3)
S1	0.0490 (12)	0.0419 (12)	0.0570 (12)	−0.0176 (10)	−0.0044 (9)	−0.0086 (10)
C1	0.042 (4)	0.041 (4)	0.031 (4)	−0.028 (4)	0.000 (3)	0.001 (3)
C2	0.046 (4)	0.036 (4)	0.035 (4)	−0.023 (4)	0.000 (3)	−0.002 (3)
C3	0.050 (5)	0.044 (5)	0.036 (4)	−0.026 (4)	0.010 (3)	−0.007 (3)
C4	0.067 (5)	0.067 (6)	0.043 (5)	−0.046 (5)	0.010 (4)	−0.014 (4)
C5	0.091 (7)	0.077 (7)	0.044 (5)	−0.062 (6)	0.022 (5)	−0.026 (5)
C6	0.113 (8)	0.053 (6)	0.059 (6)	−0.050 (6)	0.036 (6)	−0.028 (5)
C7	0.081 (6)	0.053 (6)	0.069 (6)	−0.014 (5)	0.014 (5)	−0.021 (5)
C8	0.076 (6)	0.057 (6)	0.051 (5)	−0.031 (5)	0.007 (4)	−0.017 (4)
C9	0.037 (4)	0.031 (4)	0.029 (4)	−0.014 (3)	−0.009 (3)	0.004 (3)
C10	0.044 (5)	0.063 (5)	0.061 (5)	−0.031 (4)	0.004 (4)	−0.012 (4)
C11	0.047 (5)	0.078 (7)	0.091 (7)	−0.047 (5)	0.001 (5)	0.004 (5)
C12	0.051 (5)	0.083 (7)	0.073 (6)	−0.036 (5)	0.016 (5)	0.004 (5)
C13	0.066 (6)	0.083 (7)	0.056 (6)	−0.029 (5)	0.027 (5)	−0.022 (5)
C14	0.047 (5)	0.049 (5)	0.047 (5)	−0.026 (4)	0.008 (4)	−0.011 (4)
C15	0.025 (3)	0.037 (4)	0.030 (4)	−0.014 (3)	0.007 (3)	−0.012 (3)
C16	0.042 (4)	0.045 (5)	0.059 (5)	−0.019 (4)	−0.015 (4)	−0.004 (4)
C17	0.075 (6)	0.043 (5)	0.070 (6)	−0.032 (5)	−0.016 (5)	0.007 (4)

C18	0.087 (7)	0.065 (6)	0.066 (6)	−0.055 (6)	−0.004 (5)	−0.009 (5)
C19	0.050 (5)	0.076 (7)	0.081 (6)	−0.039 (5)	−0.014 (5)	−0.012 (5)
C20	0.041 (4)	0.049 (5)	0.061 (5)	−0.024 (4)	−0.012 (4)	−0.002 (4)
C21	0.031 (4)	0.033 (4)	0.043 (4)	−0.018 (3)	−0.003 (3)	−0.004 (3)
C22	0.042 (4)	0.059 (5)	0.036 (4)	−0.016 (4)	−0.004 (3)	0.003 (4)
C23	0.076 (7)	0.069 (6)	0.052 (5)	−0.023 (5)	−0.024 (5)	0.024 (5)
C24	0.042 (5)	0.069 (6)	0.084 (7)	−0.001 (5)	−0.014 (5)	0.006 (6)
C25	0.043 (5)	0.063 (6)	0.072 (6)	−0.005 (4)	0.004 (4)	0.003 (5)
C26	0.035 (4)	0.051 (5)	0.054 (5)	−0.011 (4)	0.007 (4)	0.007 (4)

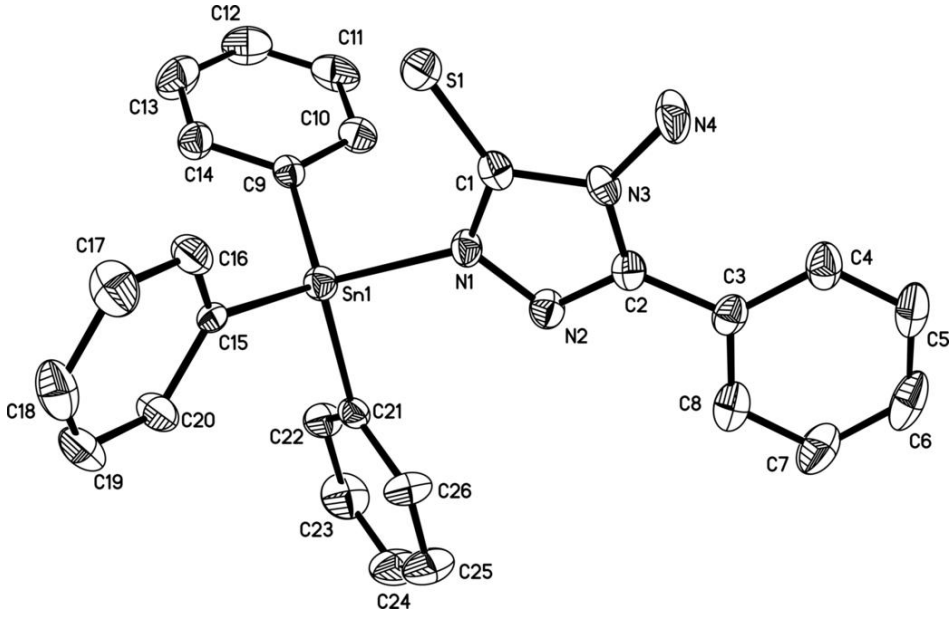
Geometric parameters (Å, °)

Sn1—N1	2.107 (5)	C11—C12	1.375 (11)
Sn1—C9	2.119 (6)	C11—H11	0.9300
Sn1—C15	2.120 (6)	C12—C13	1.349 (11)
Sn1—C21	2.133 (6)	C12—H12	0.9300
N1—C1	1.322 (8)	C13—C14	1.366 (10)
N1—N2	1.391 (7)	C13—H13	0.9300
N2—C2	1.307 (8)	C14—H14	0.9300
N3—C2	1.354 (8)	C15—C16	1.379 (9)
N3—C1	1.387 (7)	C15—C20	1.380 (9)
N3—N4	1.401 (7)	C16—C17	1.366 (10)
N4—H4A	0.860	C16—H16	0.9300
N4—H4B	0.860	C17—C18	1.360 (11)
S1—C1	1.660 (7)	C17—H17	0.9300
C2—C3	1.474 (9)	C18—C19	1.350 (11)
C3—C8	1.357 (10)	C18—H18	0.9300
C3—C4	1.379 (9)	C19—C20	1.368 (10)
C4—C5	1.360 (9)	C19—H19	0.9300
C4—H4	0.9300	C20—H20	0.9300
C5—C6	1.358 (12)	C21—C22	1.371 (9)
C5—H5	0.9300	C21—C26	1.379 (9)
C6—C7	1.371 (11)	C22—C23	1.383 (10)
C6—H6	0.9300	C22—H22	0.9300
C7—C8	1.378 (10)	C23—C24	1.364 (11)
C7—H7	0.9300	C23—H23	0.9300
C8—H8	0.9300	C24—C25	1.356 (12)
C9—C10	1.360 (9)	C24—H24	0.9300
C9—C14	1.384 (8)	C25—C26	1.369 (10)
C10—C11	1.381 (10)	C25—H25	0.9300
C10—H10	0.9300	C26—H26	0.9300
N1—Sn1—C9	105.3 (2)	C12—C11—H11	119.7
N1—Sn1—C15	110.6 (2)	C10—C11—H11	119.7
C9—Sn1—C15	119.5 (2)	C13—C12—C11	118.9 (7)
N1—Sn1—C21	99.9 (2)	C13—C12—H12	120.5
C9—Sn1—C21	110.3 (3)	C11—C12—H12	120.5
C15—Sn1—C21	109.4 (2)	C12—C13—C14	120.8 (8)
C1—N1—N2	112.5 (5)	C12—C13—H13	119.6
C1—N1—Sn1	127.6 (4)	C14—C13—H13	119.6

N2—N1—Sn1	119.8 (4)	C13—C14—C9	121.2 (7)
C2—N2—N1	105.0 (5)	C13—C14—H14	119.4
C2—N3—C1	109.3 (5)	C9—C14—H14	119.4
C2—N3—N4	128.1 (5)	C16—C15—C20	117.3 (6)
C1—N3—N4	122.5 (6)	C16—C15—Sn1	125.1 (4)
N3—N4—H4A	120.0	C20—C15—Sn1	117.4 (5)
N3—N4—H4B	120.0	C17—C16—C15	120.8 (6)
H4A—N4—H4B	120.0	C17—C16—H16	119.6
N1—C1—N3	103.4 (6)	C15—C16—H16	119.6
N1—C1—S1	127.9 (5)	C18—C17—C16	121.2 (8)
N3—C1—S1	128.6 (5)	C18—C17—H17	119.4
N2—C2—N3	109.8 (5)	C16—C17—H17	119.4
N2—C2—C3	121.0 (6)	C19—C18—C17	118.5 (7)
N3—C2—C3	129.2 (6)	C19—C18—H18	120.7
C8—C3—C4	116.2 (7)	C17—C18—H18	120.7
C8—C3—C2	118.0 (6)	C18—C19—C20	121.4 (7)
C4—C3—C2	125.6 (7)	C18—C19—H19	119.3
C5—C4—C3	122.2 (8)	C20—C19—H19	119.3
C5—C4—H4	118.9	C19—C20—C15	120.7 (7)
C3—C4—H4	118.9	C19—C20—H20	119.6
C6—C5—C4	120.7 (8)	C15—C20—H20	119.6
C6—C5—H5	119.6	C22—C21—C26	119.2 (6)
C4—C5—H5	119.6	C22—C21—Sn1	120.5 (5)
C5—C6—C7	118.5 (7)	C26—C21—Sn1	120.3 (5)
C5—C6—H6	120.8	C21—C22—C23	120.0 (7)
C7—C6—H6	120.8	C21—C22—H22	120.0
C6—C7—C8	119.9 (9)	C23—C22—H22	120.0
C6—C7—H7	120.1	C24—C23—C22	119.9 (8)
C8—C7—H7	120.1	C24—C23—H23	120.1
C3—C8—C7	122.5 (8)	C22—C23—H23	120.1
C3—C8—H8	118.8	C25—C24—C23	120.3 (8)
C7—C8—H8	118.8	C25—C24—H24	119.8
C10—C9—C14	117.9 (6)	C23—C24—H24	119.8
C10—C9—Sn1	121.3 (5)	C24—C25—C26	120.3 (8)
C14—C9—Sn1	120.7 (5)	C24—C25—H25	119.8
C9—C10—C11	120.7 (7)	C26—C25—H25	119.8
C9—C10—H10	119.7	C25—C26—C21	120.2 (7)
C11—C10—H10	119.7	C25—C26—H26	119.9
C12—C11—C10	120.5 (7)	C21—C26—H26	119.9
C9—Sn1—N1—C1	71.0 (6)	C15—Sn1—C9—C14	−21.9 (6)
C15—Sn1—N1—C1	−59.4 (6)	C21—Sn1—C9—C14	106.2 (6)
C21—Sn1—N1—C1	−174.6 (5)	C14—C9—C10—C11	−0.5 (11)
C9—Sn1—N1—N2	−111.5 (5)	Sn1—C9—C10—C11	176.6 (6)
C15—Sn1—N1—N2	118.1 (5)	C9—C10—C11—C12	0.3 (12)
C21—Sn1—N1—N2	2.9 (5)	C10—C11—C12—C13	0.3 (13)
C1—N1—N2—C2	0.4 (7)	C11—C12—C13—C14	−0.5 (14)
Sn1—N1—N2—C2	−177.5 (4)	C12—C13—C14—C9	0.2 (13)
N2—N1—C1—N3	−0.5 (7)	C10—C9—C14—C13	0.3 (11)
Sn1—N1—C1—N3	177.1 (4)	Sn1—C9—C14—C13	−176.9 (6)

N2—N1—C1—S1	175.9 (5)	N1—Sn1—C15—C16	48.9 (6)
Sn1—N1—C1—S1	−6.4 (9)	C9—Sn1—C15—C16	−73.5 (6)
C2—N3—C1—N1	0.5 (7)	C21—Sn1—C15—C16	158.0 (5)
N4—N3—C1—N1	−179.0 (5)	N1—Sn1—C15—C20	−126.6 (5)
C2—N3—C1—S1	−176.0 (5)	C9—Sn1—C15—C20	111.0 (5)
N4—N3—C1—S1	4.5 (9)	C21—Sn1—C15—C20	−17.5 (6)
N1—N2—C2—N3	−0.1 (7)	C20—C15—C16—C17	0.1 (10)
N1—N2—C2—C3	−179.2 (6)	Sn1—C15—C16—C17	−175.5 (5)
C1—N3—C2—N2	−0.2 (7)	C15—C16—C17—C18	0.0 (12)
N4—N3—C2—N2	179.3 (6)	C16—C17—C18—C19	−0.4 (13)
C1—N3—C2—C3	178.8 (6)	C17—C18—C19—C20	0.6 (13)
N4—N3—C2—C3	−1.7 (11)	C18—C19—C20—C15	−0.5 (12)
N2—C2—C3—C8	−14.5 (10)	C16—C15—C20—C19	0.2 (10)
N3—C2—C3—C8	166.6 (7)	Sn1—C15—C20—C19	176.0 (5)
N2—C2—C3—C4	160.5 (7)	N1—Sn1—C21—C22	−132.2 (5)
N3—C2—C3—C4	−18.4 (11)	C9—Sn1—C21—C22	−21.7 (6)
C8—C3—C4—C5	−1.5 (11)	C15—Sn1—C21—C22	111.7 (5)
C2—C3—C4—C5	−176.6 (7)	N1—Sn1—C21—C26	48.3 (6)
C3—C4—C5—C6	3.0 (12)	C9—Sn1—C21—C26	158.8 (5)
C4—C5—C6—C7	−3.0 (13)	C15—Sn1—C21—C26	−67.8 (6)
C5—C6—C7—C8	1.6 (13)	C26—C21—C22—C23	−1.6 (10)
C4—C3—C8—C7	0.1 (12)	Sn1—C21—C22—C23	178.9 (6)
C2—C3—C8—C7	175.6 (7)	C21—C22—C23—C24	1.6 (12)
C6—C7—C8—C3	−0.1 (14)	C22—C23—C24—C25	−1.2 (14)
N1—Sn1—C9—C10	36.1 (6)	C23—C24—C25—C26	0.9 (14)
C15—Sn1—C9—C10	161.1 (5)	C24—C25—C26—C21	−0.9 (12)
C21—Sn1—C9—C10	−70.9 (6)	C22—C21—C26—C25	1.3 (10)
N1—Sn1—C9—C14	−146.9 (5)	Sn1—C21—C26—C25	−179.2 (6)

Fig. 1


C12
C11
S1
C13
C10
N4
C14
C9
C1
N3
C17
C16
N1
C4
Sn1
C2
C3
C15
N2
C5
C18
C20
C21
C8
C22
C6
C19
C26
C7
C23
C25
C24