

(4-Chloro-3,5-dinitrobenzoato)triphenyltin(IV)

Aziz-ur-Rehman,^a Madeleine Helliwell,^b Saqib Ali^{a*} and Saira Shahzadi^a^aDepartment of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, and^bSchool of Chemistry, The University of Manchester, Manchester M13 9PL, England

Correspondence e-mail: drsa54@yahoo.com

Key indicators

Single-crystal X-ray study

T = 100 K

Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$

R factor = 0.026

wR factor = 0.068

Data-to-parameter ratio = 15.1

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

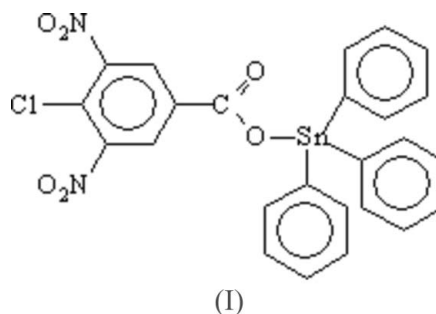
The geometry around the Sn atom of the title compound, $[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_7\text{H}_2\text{ClN}_2\text{O}_6)]$, is distorted tetrahedral, with Sn—C distances lying in the range 2.124 (2)–2.119 (2) Å and an Sn—O distance of 2.0645 (15) Å.

Received 9 June 2006

Accepted 20 June 2006

Comment

Organotin compounds are of current interest due to their dramatic increase of industrial, agricultural and biological applications (Xie *et al.*, 1996; Nath *et al.*, 2001). Studies of organotin and biologically important ligands have gained importance due to potential pharmaceutical applications of organotin compounds (Anderson *et al.*, 1984). The biological applications of organotin compounds as antitumor and anticancer agents (Yang & Guo, 1999; Gielen *et al.*, 2002) and the structural aspects of organotin carboxylates have been well documented (Tiekink, 1994; Hans *et al.*, 2002).



We report here the crystal structure of the title compound, (I), as a continuation of our efforts in the synthesis and structural characterization of organotin(IV) carboxylates (Sadiq-ur-Rehman *et al.*, 2006).

The structure of (I) is composed of discrete monomeric molecules in which the O atom of the carboxylate ligand and three C atoms of three phenyl groups surround the tetra-coordinated Sn atom (Fig. 1). The Sn atom exists in a distorted tetrahedral geometry. The largest distortion from the ideal tetrahedral geometry is found in the O1—Sn—C8 angle (Table 1); the C14—Sn1—C20 angle shows the next largest distortion from the ideal geometry. The monodentate mode of coordination of the 4-chloro-3,5-dinitrobenzoate is reflected in the disparate O1—C1 and O2—C2 bond distances, with the longer bond associated with the stronger Sn1—O1 interaction. The bond distances and angles involving the Sn atom are in agreement with the corresponding values found for similar Sn complexes (Sadiq-ur-Rehman *et al.*, 2005).

Experimental

Triphenyltin(IV) hydroxide (0.6 g, 2.4 mmol) and 3,5-dinitro-4-chlorobenzoic acid (0.9 g, 2.4 mmol) were suspended in dry toluene (150 ml) in a two-necked round-bottomed flask equipped with a water condenser. The mixture was refluxed for 8–10 h and the water that formed during the condensation reaction was periodically removed *via* a Dean–Stark separator. The mixture was cooled to room temperature and solvent was removed on a rotary evaporator under reduced pressure. The solid product was recrystallized from chloroform to obtain colourless crystals suitable for X-ray analysis (yield 75%; m.p. 414–416 K).

Crystal data

[Sn(C ₆ H ₅) ₃ (C ₇ H ₂ ClN ₂ O ₆)]	<i>Z</i> = 4
<i>M_r</i> = 595.55	<i>D_x</i> = 1.698 Mg m ⁻³
Monoclinic, <i>P</i> 2 ₁ / <i>c</i>	Mo <i>K</i> α radiation
<i>a</i> = 12.7457 (8) Å	<i>μ</i> = 1.26 mm ⁻¹
<i>b</i> = 8.3919 (5) Å	<i>T</i> = 100 (2) K
<i>c</i> = 22.3719 (14) Å	Block, colourless
<i>β</i> = 103.1560 (10)°	0.40 × 0.35 × 0.35 mm
<i>V</i> = 2330.1 (2) Å ³	

Data collection

Bruker SMART CCD area-detector diffractometer	13029 measured reflections
<i>φ</i> and <i>ω</i> scans	4757 independent reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2001)	4272 reflections with <i>I</i> > 2σ(<i>I</i>)
<i>T</i> _{min} = 0.633, <i>T</i> _{max} = 0.668	<i>R</i> _{int} = 0.029
	<i>θ</i> _{max} = 26.4°

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 1.1522P]$
$R[F^2 > 2\sigma(F^2)] = 0.026$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.068$	(Δ/σ) _{max} = 0.001
<i>S</i> = 1.03	$\Delta\rho_{\text{max}} = 1.25 \text{ e } \text{Å}^{-3}$
4757 reflections	$\Delta\rho_{\text{min}} = -0.35 \text{ e } \text{Å}^{-3}$
316 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

Sn1—O1	2.0654 (15)	Sn1—C8	2.124 (2)
Sn1—C14	2.119 (2)	O1—C1	1.305 (3)
Sn1—C20	2.120 (2)	O2—C1	1.221 (3)
O1—Sn1—C14	110.48 (7)	O1—Sn1—C8	97.64 (7)
O1—Sn1—C20	103.46 (7)	C14—Sn1—C8	111.21 (8)
C14—Sn1—C20	119.25 (9)	C20—Sn1—C8	112.28 (9)

H atoms were included in calculated positions and refined as riding, with C—H distances of 0.95 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C). The highest density peak is located 0.11 Å from atom H10.

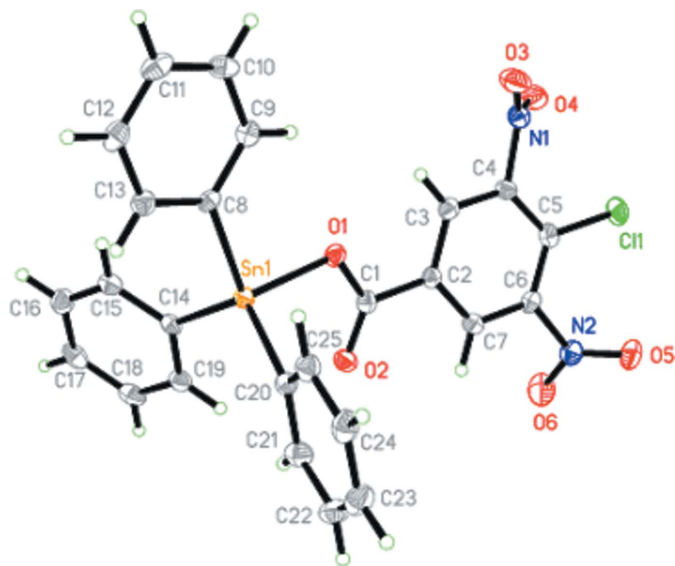


Figure 1

The structure of (I), with displacement ellipsoids drawn at the 50% probability level.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

AR is thankful to HEC (Higher Education Commission, Islamabad, Pakistan) for financial support under PhD Fellowship Scheme Batch-II (PIN Code: 042-111621-PS2-179).

References

- Anderson, K. E., Simionatto, C. S., Drummond, G. S. & Kappas, A. (1984). *J. Pharmacol. Exp. Ther.* **228**, 327–333.
- Bruker (2001). *SMART* (Version 5.625), *SADABS* (Version 2.03a) and *SHELXTL* (Version 6.12). Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2002). *SAINT*. Version 6.36a. Bruker AXS Inc., Madison, Wisconsin, USA.
- Gielen, M. (2002). *Appl. Organomet. Chem.* **16**, 481–494.
- Hans, K., Parvez, M., Ahmad, F., Ali, S., Mazhar, M. & Munir, A. (2002). *Acta Cryst. E* **58**, m441–m443.
- Nath, M., Pokharia, S. & Yadav, R. (2001). *Coord. Chem. Rev.* **215**, 99–149.
- Sadiq-ur-Rehman, Ali, S., Shahzadi, S. & Parvez, M. (2006). *Acta Cryst. E* **62**, m910–m911.
- Sadiq-ur-Rehman, Shahid, K., Ali, S., Bhatti, M. H. & Parvez, M. (2005). *J. Organomet. Chem.* **690**, 1396–1408.
- Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
- Tiekink, E. R. T. (1994). *Trends Organomet. Chem.* **1**, 71–116.
- Xie, Q., Yang, Z. & Jiang, L. (1996). *Main Group Met. Chem.* **19**, 509–520.
- Yang, P. & Guo, M. (1999). *Coord. Chem. Rev.* **185–186**, 189–211.

supporting information

Acta Cryst. (2006). E62, m1656–m1657 [https://doi.org/10.1107/S1600536806023580]

(4-Chloro-3,5-dinitrobenzoato)triphenyltin(IV)

Aziz-ur-Rehman, Madeleine Helliwell, Saqib Ali and Saira Shahzadi

(4-Chloro-3,5-dinitrobenzoato)triphenyltin(IV)

Crystal data

[Sn(C₆H₅)₃(C₇H₂ClN₂O₆)]

$M_r = 595.55$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 12.7457$ (8) Å

$b = 8.3919$ (5) Å

$c = 22.3719$ (14) Å

$\beta = 103.156$ (1)°

$V = 2330.1$ (2) Å³

$Z = 4$

$F(000) = 1184$

$D_x = 1.698$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 6521 reflections

$\theta = 2.6$ – 26.4 °

$\mu = 1.26$ mm⁻¹

$T = 100$ K

Block, colourless

$0.40 \times 0.35 \times 0.35$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2001)

$T_{\min} = 0.633$, $T_{\max} = 0.668$

13029 measured reflections

4757 independent reflections

4272 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 26.4$ °, $\theta_{\min} = 1.6$ °

$h = -15 \rightarrow 15$

$k = -10 \rightarrow 10$

$l = -27 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.026$

$wR(F^2) = 0.068$

$S = 1.03$

4757 reflections

316 parameters

0 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

$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 1.1522P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.25$ e Å⁻³

$\Delta\rho_{\min} = -0.35$ e Å⁻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 $F^2 > \sigma(F^2)$ 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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.134882 (11)	1.067962 (17)	0.129275 (7)	0.01438 (6)
Cl1	0.55398 (5)	0.72259 (8)	-0.10026 (3)	0.02763 (14)
O1	0.21016 (12)	0.99775 (19)	0.06102 (7)	0.0171 (3)
O2	0.31794 (13)	0.8587 (2)	0.13545 (7)	0.0211 (4)
O3	0.28596 (16)	0.9951 (3)	-0.14633 (9)	0.0394 (5)
O4	0.32670 (17)	0.7534 (3)	-0.16759 (9)	0.0416 (5)
O5	0.70083 (13)	0.7399 (2)	0.02386 (9)	0.0290 (4)
O6	0.62699 (16)	0.5697 (2)	0.07485 (11)	0.0387 (5)
N1	0.32621 (17)	0.8642 (3)	-0.13270 (10)	0.0264 (5)
N2	0.62382 (16)	0.6807 (2)	0.03893 (10)	0.0215 (4)
C1	0.29240 (18)	0.9052 (3)	0.08239 (11)	0.0162 (5)
C2	0.35596 (17)	0.8602 (3)	0.03634 (10)	0.0157 (4)
C3	0.31641 (18)	0.8872 (3)	-0.02591 (11)	0.0176 (5)
H3	0.2485	0.9375	-0.0401	0.021*
C4	0.37641 (18)	0.8404 (3)	-0.06694 (10)	0.0187 (5)
C5	0.47870 (18)	0.7729 (3)	-0.04867 (11)	0.0189 (5)
C6	0.51593 (17)	0.7503 (3)	0.01411 (11)	0.0169 (5)
C7	0.45593 (18)	0.7886 (3)	0.05622 (11)	0.0172 (5)
H7	0.4829	0.7660	0.0985	0.021*
C8	0.01540 (17)	1.2159 (3)	0.07450 (10)	0.0155 (4)
C9	0.00488 (18)	1.2329 (3)	0.01143 (11)	0.0185 (5)
H9	0.0518	1.1761	-0.0084	0.022*
C10	-0.07344 (19)	1.3319 (3)	-0.02249 (11)	0.0221 (5)
H10	-0.0801	1.3424	-0.0655	0.026*
C11	-0.1419 (2)	1.4156 (3)	0.00592 (12)	0.0230 (5)
H11	-0.1955	1.4834	-0.0175	0.028*
C12	-0.13241 (19)	1.4007 (3)	0.06854 (12)	0.0232 (5)
H12	-0.1795	1.4581	0.0881	0.028*
C13	-0.05419 (18)	1.3018 (3)	0.10265 (11)	0.0205 (5)
H13	-0.0477	1.2922	0.1456	0.025*
C14	0.06444 (18)	0.8692 (3)	0.16362 (10)	0.0161 (4)
C15	-0.04809 (18)	0.8590 (3)	0.15001 (11)	0.0190 (5)
H15	-0.0899	0.9365	0.1241	0.023*
C16	-0.0992 (2)	0.7363 (3)	0.17408 (11)	0.0239 (5)
H16	-0.1756	0.7306	0.1649	0.029*
C17	-0.0382 (2)	0.6224 (3)	0.21159 (11)	0.0239 (5)
H17	-0.0730	0.5377	0.2276	0.029*
C18	0.0729 (2)	0.6319 (3)	0.22562 (11)	0.0242 (5)
H18	0.1142	0.5540	0.2516	0.029*
C19	0.12474 (19)	0.7545 (3)	0.20213 (11)	0.0201 (5)

H19	0.2012	0.7605	0.2122	0.024*
C20	0.25521 (18)	1.2014 (3)	0.18982 (10)	0.0180 (5)
C21	0.32980 (19)	1.1282 (3)	0.23723 (11)	0.0231 (5)
H21	0.3233	1.0180	0.2453	0.028*
C22	0.4136 (2)	1.2166 (3)	0.27265 (12)	0.0273 (6)
H22	0.4647	1.1662	0.3046	0.033*
C23	0.4231 (2)	1.3779 (3)	0.26163 (12)	0.0286 (6)
H23	0.4813	1.4373	0.2855	0.034*
C24	0.3476 (2)	1.4524 (3)	0.21570 (12)	0.0256 (6)
H24	0.3530	1.5634	0.2087	0.031*
C25	0.26397 (19)	1.3643 (3)	0.17980 (11)	0.0213 (5)
H25	0.2125	1.4156	0.1483	0.026*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01423 (9)	0.01387 (9)	0.01520 (10)	0.00213 (5)	0.00367 (6)	-0.00005 (6)
Cl1	0.0266 (3)	0.0353 (3)	0.0252 (3)	0.0020 (2)	0.0148 (3)	-0.0049 (3)
O1	0.0144 (7)	0.0191 (8)	0.0179 (8)	0.0019 (6)	0.0042 (6)	-0.0019 (7)
O2	0.0221 (8)	0.0256 (9)	0.0162 (9)	0.0039 (7)	0.0054 (7)	0.0008 (7)
O3	0.0399 (11)	0.0546 (13)	0.0258 (11)	0.0216 (10)	0.0117 (9)	0.0147 (10)
O4	0.0493 (13)	0.0522 (13)	0.0201 (10)	-0.0002 (10)	0.0015 (9)	-0.0103 (9)
O5	0.0183 (9)	0.0301 (10)	0.0404 (11)	0.0011 (7)	0.0102 (8)	0.0025 (8)
O6	0.0314 (11)	0.0337 (11)	0.0537 (14)	0.0124 (8)	0.0149 (10)	0.0218 (9)
N1	0.0209 (10)	0.0405 (13)	0.0188 (11)	0.0035 (10)	0.0069 (8)	0.0034 (10)
N2	0.0200 (10)	0.0193 (10)	0.0259 (11)	0.0044 (8)	0.0066 (9)	-0.0011 (9)
C1	0.0167 (11)	0.0129 (10)	0.0197 (12)	-0.0028 (8)	0.0054 (9)	-0.0020 (9)
C2	0.0161 (10)	0.0141 (10)	0.0174 (11)	-0.0028 (8)	0.0048 (9)	-0.0019 (9)
C3	0.0165 (11)	0.0160 (11)	0.0198 (12)	-0.0004 (9)	0.0029 (9)	0.0008 (9)
C4	0.0204 (11)	0.0211 (12)	0.0145 (12)	-0.0024 (9)	0.0036 (9)	-0.0010 (9)
C5	0.0219 (12)	0.0155 (11)	0.0216 (12)	-0.0021 (9)	0.0096 (10)	-0.0034 (9)
C6	0.0149 (11)	0.0129 (10)	0.0228 (12)	0.0013 (8)	0.0042 (9)	-0.0010 (9)
C7	0.0198 (11)	0.0140 (10)	0.0178 (12)	-0.0006 (9)	0.0044 (9)	0.0004 (9)
C8	0.0130 (10)	0.0131 (10)	0.0193 (12)	-0.0005 (8)	0.0012 (9)	-0.0001 (9)
C9	0.0190 (11)	0.0150 (11)	0.0218 (13)	0.0001 (9)	0.0054 (9)	-0.0021 (9)
C10	0.0272 (13)	0.0182 (12)	0.0182 (12)	-0.0021 (9)	-0.0003 (10)	-0.0005 (9)
C11	0.0206 (12)	0.0145 (11)	0.0304 (14)	0.0016 (9)	-0.0015 (10)	-0.0002 (10)
C12	0.0187 (12)	0.0196 (12)	0.0311 (14)	0.0047 (9)	0.0054 (10)	-0.0038 (10)
C13	0.0189 (11)	0.0217 (12)	0.0209 (12)	0.0028 (9)	0.0044 (9)	-0.0016 (10)
C14	0.0204 (11)	0.0155 (11)	0.0136 (11)	0.0007 (9)	0.0061 (9)	-0.0012 (9)
C15	0.0225 (12)	0.0178 (11)	0.0166 (12)	0.0017 (9)	0.0043 (9)	0.0002 (9)
C16	0.0223 (12)	0.0248 (13)	0.0251 (13)	-0.0033 (9)	0.0065 (10)	-0.0021 (10)
C17	0.0362 (14)	0.0175 (12)	0.0208 (13)	-0.0039 (10)	0.0120 (11)	0.0001 (10)
C18	0.0353 (14)	0.0209 (12)	0.0163 (12)	0.0055 (10)	0.0056 (10)	0.0025 (10)
C19	0.0225 (12)	0.0214 (12)	0.0164 (12)	0.0054 (9)	0.0046 (9)	0.0014 (9)
C20	0.0166 (11)	0.0221 (11)	0.0158 (11)	0.0014 (9)	0.0046 (9)	-0.0050 (9)
C21	0.0261 (13)	0.0220 (12)	0.0205 (13)	0.0046 (10)	0.0038 (10)	-0.0030 (10)
C22	0.0232 (13)	0.0352 (15)	0.0209 (13)	0.0074 (11)	0.0000 (10)	-0.0069 (11)

C23	0.0207 (12)	0.0348 (15)	0.0295 (15)	-0.0022 (11)	0.0039 (11)	-0.0151 (12)
C24	0.0231 (13)	0.0245 (13)	0.0315 (15)	-0.0017 (10)	0.0109 (11)	-0.0071 (11)
C25	0.0198 (12)	0.0221 (12)	0.0233 (13)	0.0015 (9)	0.0074 (10)	-0.0021 (10)

Geometric parameters (Å, °)

Sn1—O1	2.0654 (15)	C11—C12	1.384 (4)
Sn1—C14	2.119 (2)	C11—H11	0.9500
Sn1—C20	2.120 (2)	C12—C13	1.385 (3)
Sn1—C8	2.124 (2)	C12—H12	0.9500
Cl1—C5	1.713 (2)	C13—H13	0.9500
O1—C1	1.305 (3)	C14—C19	1.400 (3)
O2—C1	1.221 (3)	C14—C15	1.400 (3)
O3—N1	1.221 (3)	C15—C16	1.390 (3)
O4—N1	1.215 (3)	C15—H15	0.9500
O5—N2	1.214 (3)	C16—C17	1.388 (3)
O6—N2	1.225 (3)	C16—H16	0.9500
N1—C4	1.478 (3)	C17—C18	1.382 (4)
N2—C6	1.481 (3)	C17—H17	0.9500
C1—C2	1.497 (3)	C18—C19	1.389 (3)
C2—C7	1.387 (3)	C18—H18	0.9500
C2—C3	1.387 (3)	C19—H19	0.9500
C3—C4	1.379 (3)	C20—C25	1.394 (3)
C3—H3	0.9500	C20—C21	1.395 (3)
C4—C5	1.395 (3)	C21—C22	1.391 (3)
C5—C6	1.389 (3)	C21—H21	0.9500
C6—C7	1.380 (3)	C22—C23	1.385 (4)
C7—H7	0.9500	C22—H22	0.9500
C8—C9	1.394 (3)	C23—C24	1.387 (4)
C8—C13	1.399 (3)	C23—H23	0.9500
C9—C10	1.385 (3)	C24—C25	1.392 (3)
C9—H9	0.9500	C24—H24	0.9500
C10—C11	1.382 (4)	C25—H25	0.9500
C10—H10	0.9500		
O1—Sn1—C14	110.48 (7)	C10—C11—H11	120.0
O1—Sn1—C20	103.46 (7)	C12—C11—H11	120.0
C14—Sn1—C20	119.25 (9)	C11—C12—C13	119.9 (2)
O1—Sn1—C8	97.64 (7)	C11—C12—H12	120.1
C14—Sn1—C8	111.21 (8)	C13—C12—H12	120.1
C20—Sn1—C8	112.28 (9)	C12—C13—C8	120.8 (2)
C1—O1—Sn1	111.63 (14)	C12—C13—H13	119.6
O4—N1—O3	126.2 (2)	C8—C13—H13	119.6
O4—N1—C4	118.1 (2)	C19—C14—C15	118.9 (2)
O3—N1—C4	115.6 (2)	C19—C14—Sn1	123.09 (17)
O5—N2—O6	125.8 (2)	C15—C14—Sn1	117.86 (17)
O5—N2—C6	118.34 (19)	C16—C15—C14	120.6 (2)
O6—N2—C6	115.8 (2)	C16—C15—H15	119.7

O2—C1—O1	124.1 (2)	C14—C15—H15	119.7
O2—C1—C2	121.5 (2)	C17—C16—C15	119.8 (2)
O1—C1—C2	114.4 (2)	C17—C16—H16	120.1
C7—C2—C3	119.3 (2)	C15—C16—H16	120.1
C7—C2—C1	119.4 (2)	C18—C17—C16	120.1 (2)
C3—C2—C1	121.3 (2)	C18—C17—H17	120.0
C4—C3—C2	119.5 (2)	C16—C17—H17	120.0
C4—C3—H3	120.3	C17—C18—C19	120.5 (2)
C2—C3—H3	120.3	C17—C18—H18	119.7
C3—C4—C5	122.9 (2)	C19—C18—H18	119.7
C3—C4—N1	116.4 (2)	C18—C19—C14	120.1 (2)
C5—C4—N1	120.7 (2)	C18—C19—H19	120.0
C6—C5—C4	115.7 (2)	C14—C19—H19	120.0
C6—C5—C11	122.18 (18)	C25—C20—C21	119.2 (2)
C4—C5—C11	122.16 (18)	C25—C20—Sn1	119.22 (17)
C7—C6—C5	122.9 (2)	C21—C20—Sn1	121.44 (17)
C7—C6—N2	116.6 (2)	C22—C21—C20	120.0 (2)
C5—C6—N2	120.5 (2)	C22—C21—H21	120.0
C6—C7—C2	119.6 (2)	C20—C21—H21	120.0
C6—C7—H7	120.2	C23—C22—C21	120.4 (2)
C2—C7—H7	120.2	C23—C22—H22	119.8
C9—C8—C13	118.6 (2)	C21—C22—H22	119.8
C9—C8—Sn1	122.33 (16)	C22—C23—C24	119.9 (2)
C13—C8—Sn1	119.09 (17)	C22—C23—H23	120.1
C10—C9—C8	120.5 (2)	C24—C23—H23	120.1
C10—C9—H9	119.8	C23—C24—C25	120.0 (2)
C8—C9—H9	119.8	C23—C24—H24	120.0
C11—C10—C9	120.3 (2)	C25—C24—H24	120.0
C11—C10—H10	119.9	C24—C25—C20	120.4 (2)
C9—C10—H10	119.9	C24—C25—H25	119.8
C10—C11—C12	120.0 (2)	C20—C25—H25	119.8
C14—Sn1—O1—C1	-65.67 (15)	C20—Sn1—C8—C13	-67.95 (19)
C20—Sn1—O1—C1	63.07 (16)	C13—C8—C9—C10	-0.5 (3)
C8—Sn1—O1—C1	178.24 (14)	Sn1—C8—C9—C10	-179.31 (17)
Sn1—O1—C1—O2	3.9 (3)	C8—C9—C10—C11	0.2 (3)
Sn1—O1—C1—C2	-175.42 (14)	C9—C10—C11—C12	0.0 (4)
O2—C1—C2—C7	-11.6 (3)	C10—C11—C12—C13	0.0 (4)
O1—C1—C2—C7	167.7 (2)	C11—C12—C13—C8	-0.3 (4)
O2—C1—C2—C3	167.7 (2)	C9—C8—C13—C12	0.5 (3)
O1—C1—C2—C3	-13.0 (3)	Sn1—C8—C13—C12	179.37 (18)
C7—C2—C3—C4	0.9 (3)	O1—Sn1—C14—C19	74.1 (2)
C1—C2—C3—C4	-178.4 (2)	C20—Sn1—C14—C19	-45.5 (2)
C2—C3—C4—C5	-3.1 (3)	C8—Sn1—C14—C19	-178.58 (18)
C2—C3—C4—N1	176.4 (2)	O1—Sn1—C14—C15	-110.03 (17)
O4—N1—C4—C3	-131.2 (2)	C20—Sn1—C14—C15	130.36 (17)
O3—N1—C4—C3	47.4 (3)	C8—Sn1—C14—C15	-2.7 (2)
O4—N1—C4—C5	48.3 (3)	C19—C14—C15—C16	-0.4 (3)

O3—N1—C4—C5	-133.1 (2)	Sn1—C14—C15—C16	-176.36 (18)
C3—C4—C5—C6	2.0 (3)	C14—C15—C16—C17	-0.4 (4)
N1—C4—C5—C6	-177.5 (2)	C15—C16—C17—C18	0.8 (4)
C3—C4—C5—C11	-177.46 (18)	C16—C17—C18—C19	-0.4 (4)
N1—C4—C5—C11	3.0 (3)	C17—C18—C19—C14	-0.4 (4)
C4—C5—C6—C7	1.2 (3)	C15—C14—C19—C18	0.8 (3)
C11—C5—C6—C7	-179.28 (17)	Sn1—C14—C19—C18	176.54 (17)
C4—C5—C6—N2	-179.52 (19)	O1—Sn1—C20—C25	88.62 (18)
C11—C5—C6—N2	0.0 (3)	C14—Sn1—C20—C25	-148.26 (17)
O5—N2—C6—C7	-128.6 (2)	C8—Sn1—C20—C25	-15.6 (2)
O6—N2—C6—C7	49.3 (3)	O1—Sn1—C20—C21	-87.52 (19)
O5—N2—C6—C5	52.1 (3)	C14—Sn1—C20—C21	35.6 (2)
O6—N2—C6—C5	-130.0 (2)	C8—Sn1—C20—C21	168.25 (18)
C5—C6—C7—C2	-3.4 (3)	C25—C20—C21—C22	-2.0 (4)
N2—C6—C7—C2	177.37 (19)	Sn1—C20—C21—C22	174.18 (18)
C3—C2—C7—C6	2.2 (3)	C20—C21—C22—C23	0.7 (4)
C1—C2—C7—C6	-178.5 (2)	C21—C22—C23—C24	1.1 (4)
O1—Sn1—C8—C9	2.91 (19)	C22—C23—C24—C25	-1.5 (4)
C14—Sn1—C8—C9	-112.61 (18)	C23—C24—C25—C20	0.2 (4)
C20—Sn1—C8—C9	110.89 (18)	C21—C20—C25—C24	1.5 (3)
O1—Sn1—C8—C13	-175.94 (17)	Sn1—C20—C25—C24	-174.70 (18)
C14—Sn1—C8—C13	68.55 (19)		
