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Bis(tetraphenylarsonium) tris(2-thioxo-1,3-dithiole-4,5-dithiolato)stannate(IV) acetone solvate at 120 K

Nadia M. Comerlato,[a] Glaucio B. Ferreira,[a] R. Alan Howie[b]* and James L. Wardell[a]

[a]Departamento de Química Inorgânica, Instituto de Química, Universidade Federal do Rio de Janeiro, CP 68563, 21945-970 Rio de Janeiro, RJ, Brazil, and [b]Department of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, Scotland

Correspondence e-mail: r.a.howie@abdn.ac.uk

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.006 Å
R factor = 0.045
wR factor = 0.079
Data-to-parameter ratio = 19.8

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

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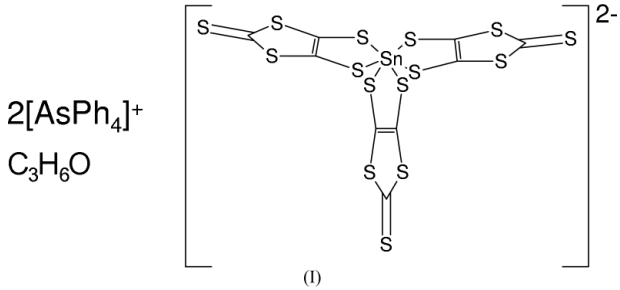
The title compound, $(C_{24}H_{20}As)_2[Sn(C_3S_5)_3]\cdot C_3H_6O$, is a further example of a salt of the general form $Q_2[Sn(dmit)_3]$ (dimit is 1,3-dithiole-2-thione-4,5-dithiolate), where Q, the onium counter-cation, is in this case $[AsPh_4]^+$. As in all such compounds, the coordination of the Sn atom is in the form of a distorted octahedron, with Sn—S distances in the range 2.5310 (10)–2.5585 (12) Å provided by three chelating dmit ligands with bite angles in the range 81.59 (3)–87.42 (3)°.

Comment

The title compound, (I), is a solvated complex salt which can be formulated as $[AsPh_4]_2[Sn(dmit)_3]\cdot Me_2CO$ and is isostructural with similarly solvated $[PPh_4]_2[Sn(dmit)_3]\cdot Me_2CO$, (II) (de Assis *et al.*, 1999), but with better refinement of the solvent molecule. Indeed, the acetone molecule was eliminated from the refinement of the structure of (II) by means of the *SQUEEZE* subroutine of *PLATON* (Spek, 2003).



(I)

The asymmetric unit of (I) consists of two $[AsPh_4]^+$ cations, the complete dianion and an acetone molecule. The anion is shown in Fig. 1 and selected bond lengths and angles within it are given in Table 1. The two cations, each with near tetrahedral As, show very small differences. Bond lengths and angles in the cations, and within the dmit ligands, are as expected. The three chelating dmit ligands are bound to the Sn atom with differing degrees of asymmetry, with Sn—S bond lengths falling in the range 2.5310 (10)–2.5585 (12) Å and chelate bite angles of 81.59 (3)–87.42 (3)°, providing distorted octahedral coordination. This situation is entirely comparable with that found in other $[Q]_2[Sn(dmit)_3]$ complexes, where Q is an onium counter-cation, such as those described by de Assis *et al.* (1999). With the dmit plane defined as that containing the C=C bond and the attached S atoms and the individual ligands defined as *L*1 (S1–S5/C1–C3), *L*2 (S6–S10/C4–C6) and *L*3 (S11–S15/C7–C9), the displacements of the Sn atom from the mean planes of the ligands are 1.1470 (16), 1.5966 (13) and −0.0362 (14) Å, respectively. These displace-

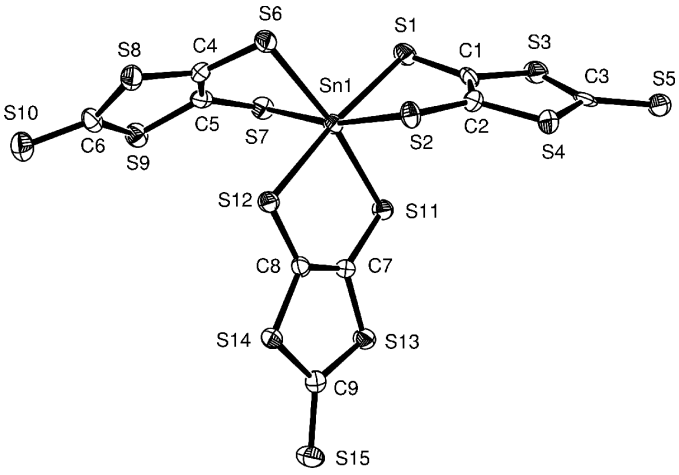


Figure 1
The anion of (I). Displacement ellipsoids are drawn at the 50% probability level.

ments correlate closely with the dihedral angles between each of the ligand planes as defined above and the plane defined, ligand by ligand, by Sn1 and the two chelating S atoms which, in the same order of the ligands as before, are 36.67 (5), 53.32 (5) and 1.15 (5)°, respectively. Thus the variation in these displacements and the corresponding dihedral angles can be ascribed to variation in tilt of the ligands about the line joining the chelating S atoms. This form of ligand tilt is clearly implicated in the wide variation in the overall shape of the $[Sn(dmit)_3]^{2-}$ dianion, ranging from T-shaped as in (I) and (II) to Y-shaped when other *Q* counter-cations are present in the structure (see *e.g.* de Assis *et al.*, 1999). The ligands also differ in the displacements from the ligand plane of their terminal thione S atoms and the C atoms to which these are attached, which fall in the ranges −0.53 (2)–0.329 (2) and −0.025 (4)–0.122 (4) Å, respectively. The completeness of the coordination (coordinative saturation) of the Sn atom precludes interanion metal–sulfur interactions, which are therefore entirely absent. The size of the counter-cations keeps the anions apart, with the result that interanion S···S contacts of any significance are also entirely absent. As would be expected, however, π–π and C—H···π interactions between the cations do occur, but these interactions are not discussed here.

Experimental

Compound (I) was obtained from a mixture of solutions of $[AsPh_4]_2[Zn(dmit)_2]$ (1.00 mmol) (Wardell *et al.*, 1997, 2000) in acetone (25 ml) and anhydrous $SnCl_4$ (0.1 ml, 0.223 g, 0.85 mmol) in MeOH (20 ml). After stirring for 1 h, the reaction mixture was filtered and the red precipitate of $[AsPh_4]_2[Sn(dmit)_3]$ was collected. Further product was isolated from the filtrate left overnight at 273 K after addition of methanol. Recrystallization of the total product, yield 80%, from Me_2CO gave the solvate, $[AsPh_4]_2[Sn(dmit)_3]\cdot Me_2CO$, m.p. 451–452 K. Analysis found: C 46.98, H 3.00%; calculated for $C_{60}H_{46}As_2OS_{15}Sn$: C 47.02, H 3.03%. IR (CsI, cm^{-1}): ν 3057, 1710, 1438, 1482, 1438, 1413, 1082, 1054, 1033, 737, 687, 477, 464, 351, 318, 280, 254, 173, 161. Raman (cm^{-1}): ν 3504, 1576, 1432, 1414, 1038, 1053, 1021, 1000, 522, 467, 348, 320, 238, 188, 173, 163.

Crystal data

$(C_{24}H_{20}As)_2[Sn(C_3S_5)_3]\cdot C_3H_6O$	$Z = 2$
$M_r = 1532.40$	$D_x = 1.625$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 11.2238$ (3) Å	Cell parameters from 20 626 reflections
$b = 14.7826$ (5) Å	$\theta = 2.9$–$27.5°$
$c = 19.9333$ (7) Å	$\mu = 2.00$ mm^{-1}
$\alpha = 99.0800$ (12)°	$T = 120$ (2) K
$\beta = 99.966$ (2)°	Rod, red
$\gamma = 101.187$ (2)°	0.36 × 0.10 × 0.03 mm
$V = 3132.15$ (17) Å^3	

Data collection

Nonius KappaCCD area-detector diffractometer	14 151 independent reflections
φ and ω scans	8442 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)	$R_{int} = 0.074$
$T_{min} = 0.891$, $T_{max} = 0.943$	$\theta_{max} = 27.5°$
43 056 measured reflections	$h = -14 \rightarrow 14$
	$k = -19 \rightarrow 19$
	$l = -25 \rightarrow 25$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.045$	$w = 1/[\sigma^2(F_o^2) + (0.0212P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.079$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.93$	$\Delta\rho_{max} = 0.90$ e Å^{-3}
14151 reflections	$\Delta\rho_{min} = -0.79$ e Å^{-3}
714 parameters	

Table 1
Selected geometric parameters (Å, °).

Sn1—S12	2.5310 (10)	Sn1—S7	2.5517 (10)
Sn1—S11	2.5320 (11)	Sn1—S2	2.5553 (10)
Sn1—S1	2.5503 (10)	Sn1—S6	2.5585 (12)
S12—Sn1—S11	87.42 (3)	S1—Sn1—S2	82.97 (3)
S12—Sn1—S1	173.46 (3)	S7—Sn1—S2	167.34 (4)
S11—Sn1—S1	89.51 (3)	S12—Sn1—S6	86.64 (3)
S12—Sn1—S7	96.99 (3)	S11—Sn1—S6	171.55 (3)
S11—Sn1—S7	93.20 (4)	S1—Sn1—S6	97.00 (4)
S1—Sn1—S7	88.95 (3)	S7—Sn1—S6	81.59 (3)
S12—Sn1—S2	91.63 (3)	S2—Sn1—S6	89.70 (3)
S11—Sn1—S2	96.46 (3)		

In the final stages of refinement H atoms were placed in calculated positions, with C—H = 0.95 and 0.98 Å for aryl and methyl H atoms, respectively, and refined with a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$ for aryl H atoms and $1.5U_{eq}(C)$ for methyl H atoms.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2003).

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Triclinic, $P\overline{1}$
Hall symbol: -P 1
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$\gamma = 101.187\ (2)°$
$V = 3132.15\ (17)$ Å^3
$Z = 2$
$F(000) = 1540$
$D_x = 1.625$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 20626 reflections
$\theta = 2.9–27.5°$
$\mu = 2.00$ mm^{-1}
$T = 120$ K
Rod, red
0.36 × 0.10 × 0.03 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: Enraf–Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans to fill the Ewald sphere
Absorption correction: multi-scan (SORTAV; Blessing, 1995, 1997)
$T_{min} = 0.891$, $T_{max} = 0.943$
43056 measured reflections
14151 independent reflections
8442 reflections with $I > 2\sigma(I)$
$R_{int} = 0.074$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -14\rightarrow14$
$k = -19\rightarrow19$
$l = -25\rightarrow25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.079$
$S = 0.93$
14151 reflections
714 parameters
0 restraints
Primary atom site location: heavy-atom method
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0212P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.90$ e Å^{-3}
$\Delta\rho_{min} = -0.79$ 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.
Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)
1.0346 (0.0052) *x* + 9.6427 (0.0044) *y* + 10.9656 (0.0074) *z* = 6.2634 (0.0015)
* -0.0095 (0.0013) S1 * 0.0198 (0.0013) S2 * -0.0057 (0.0032) C1 * -0.0139 (0.0033) C2 * 0.0199 (0.0012) S3 * -0.0107 (0.0012) S4 - 0.0252 (0.0043) C3 - 0.0533 (0.0023) S5 1.1470 (0.0016) Sn1
Rms deviation of fitted atoms = 0.0143
9.5094 (0.0026) *x* + 3.5555 (0.0052) *y* + 1.9069 (0.0087) *z* = 3.5553 (0.0030)
Angle to previous plane (with approximate e.s.d.) = 52.96 (0.04)
* 0.0514 (0.0011) S6 * 0.0391 (0.0011) S7 * -0.0821 (0.0030) C4 * -0.0901 (0.0029) C5 * 0.0314 (0.0011) S8 * 0.0503 (0.0011) S9 0.1219 (0.0039) C6 0.3287 (0.0020) S10 1.5966 (0.0013) Sn1
Rms deviation of fitted atoms = 0.0613
- 9.7786 (0.0018) *x* + 9.2006 (0.0041) *y* + 4.3916 (0.0077) *z* = 2.3615 (0.0036)
Angle to previous plane (with approximate e.s.d.) = 60.52 (0.02)
* -0.0093 (0.0011) S11 * 0.0082 (0.0011) S12 * -0.0019 (0.0028) C7 * 0.0040 (0.0027) C8 * 0.0116 (0.0010) S13 * -0.0126 (0.0010) S14 0.0237 (0.0036) C9 0.0557 (0.0019) S15 - 0.0362 (0.0014) Sn1
Rms deviation of fitted atoms = 0.0088

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. Anisotropic displacement parameters refined for all non-H including those of the solvent acetone molecule. In the final stages H introduced in calculated positions and refined with a riding model. Rotational orientation of rigid body Me groups also refined.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.31660 (2)	0.484116 (19)	0.220202 (15)	0.01932 (8)
S1	0.22146 (9)	0.33307 (7)	0.25654 (6)	0.0258 (3)
S2	0.47220 (9)	0.38963 (7)	0.18582 (6)	0.0241 (3)
C1	0.3590 (3)	0.2966 (3)	0.2760 (2)	0.0215 (10)
C2	0.4597 (3)	0.3184 (3)	0.2466 (2)	0.0223 (10)
S3	0.37496 (9)	0.22662 (8)	0.33834 (6)	0.0305 (3)
S4	0.58592 (9)	0.27134 (7)	0.27632 (6)	0.0281 (3)
C3	0.5232 (3)	0.2111 (3)	0.3339 (2)	0.0270 (10)
S5	0.59587 (10)	0.14739 (8)	0.38049 (7)	0.0389 (3)
S6	0.19519 (9)	0.44182 (7)	0.09420 (6)	0.0257 (3)
S7	0.12576 (9)	0.54656 (7)	0.23877 (6)	0.0256 (3)
C4	0.1407 (3)	0.5454 (3)	0.1029 (2)	0.0240 (10)
C5	0.1125 (3)	0.5869 (3)	0.1616 (2)	0.0228 (10)
S8	0.14237 (9)	0.60875 (8)	0.03591 (6)	0.0288 (3)
S9	0.08514 (9)	0.70003 (7)	0.16099 (6)	0.0286 (3)
C6	0.1066 (3)	0.7081 (3)	0.0766 (2)	0.0276 (11)
S10	0.09939 (10)	0.80286 (8)	0.04425 (7)	0.0362 (3)
S11	0.43187 (9)	0.55017 (7)	0.34460 (6)	0.0231 (2)
S12	0.43487 (9)	0.62976 (7)	0.18853 (6)	0.0232 (3)
C7	0.5226 (3)	0.6537 (3)	0.3316 (2)	0.0198 (9)

C8	0.5233 (3)	0.6841 (3)	0.2705 (2)	0.0201 (10)
S13	0.62314 (9)	0.72711 (7)	0.40456 (6)	0.0260 (3)
S14	0.62818 (9)	0.79085 (7)	0.27672 (6)	0.0225 (2)
C9	0.6866 (3)	0.8149 (3)	0.3648 (2)	0.0219 (10)
S15	0.79269 (10)	0.91093 (8)	0.40699 (6)	0.0335 (3)
As1	0.10599 (3)	0.68939 (3)	0.45402 (2)	0.01758 (10)
C10	0.1910 (3)	0.5913 (3)	0.4662 (2)	0.0162 (9)
C11	0.1458 (3)	0.5016 (3)	0.4263 (2)	0.0207 (10)
H11	0.0712	0.4874	0.3919	0.025*
C12	0.2115 (3)	0.4325 (3)	0.4373 (2)	0.0245 (10)
H12	0.1818	0.3708	0.4100	0.029*
C13	0.3197 (4)	0.4532 (3)	0.4876 (2)	0.0261 (11)
H13	0.3631	0.4055	0.4955	0.031*
C14	0.3646 (3)	0.5435 (3)	0.5265 (2)	0.0238 (10)
H14	0.4391	0.5577	0.5609	0.029*
C15	0.3018 (3)	0.6127 (3)	0.5156 (2)	0.0210 (10)
H15	0.3337	0.6750	0.5417	0.025*
C16	0.2186 (3)	0.7909 (3)	0.4335 (2)	0.0177 (9)
C17	0.2347 (3)	0.8822 (3)	0.4695 (2)	0.0224 (10)
H17	0.1884	0.8957	0.5040	0.027*
C18	0.3201 (3)	0.9534 (3)	0.4542 (2)	0.0271 (10)
H18	0.3321	1.0165	0.4779	0.033*
C19	0.3876 (3)	0.9322 (3)	0.4045 (2)	0.0250 (10)
H19	0.4478	0.9807	0.3952	0.030*
C20	0.3683 (3)	0.8420 (3)	0.3685 (2)	0.0271 (11)
H20	0.4137	0.8290	0.3335	0.032*
C21	0.2842 (3)	0.7699 (3)	0.3823 (2)	0.0220 (10)
H21	0.2713	0.7073	0.3573	0.026*
C22	0.0522 (3)	0.7332 (3)	0.5365 (2)	0.0189 (9)
C23	−0.0309 (3)	0.7916 (3)	0.5315 (2)	0.0243 (10)
H23	−0.0622	0.8057	0.4879	0.029*
C24	−0.0678 (4)	0.8291 (3)	0.5907 (3)	0.0323 (11)
H24	−0.1246	0.8690	0.5879	0.039*
C25	−0.0216 (4)	0.8081 (3)	0.6538 (2)	0.0322 (11)
H25	−0.0454	0.8351	0.6944	0.039*
C26	0.0586 (4)	0.7484 (3)	0.6587 (2)	0.0306 (11)
H26	0.0872	0.7325	0.7021	0.037*
C27	0.0973 (3)	0.7118 (3)	0.5998 (2)	0.0221 (10)
H27	0.1544	0.6722	0.6029	0.027*
C28	−0.0362 (3)	0.6461 (3)	0.3802 (2)	0.0162 (9)
C29	−0.0462 (3)	0.6898 (3)	0.3233 (2)	0.0205 (10)
H29	0.0174	0.7415	0.3212	0.025*
C30	−0.1498 (3)	0.6573 (3)	0.2697 (2)	0.0266 (10)
H30	−0.1582	0.6871	0.2308	0.032*
C31	−0.2410 (3)	0.5813 (3)	0.2729 (2)	0.0279 (11)
H31	−0.3112	0.5581	0.2356	0.033*
C32	−0.2308 (3)	0.5389 (3)	0.3297 (2)	0.0246 (10)
H32	−0.2944	0.4871	0.3314	0.030*

C33	−0.1292 (3)	0.5712 (3)	0.3841 (2)	0.0227 (10)
H33	−0.1229	0.5425	0.4236	0.027*
As2	0.22529 (3)	−0.01399 (3)	0.87463 (2)	0.01908 (11)
C34	0.3772 (3)	0.0369 (3)	0.8490 (2)	0.0206 (10)
C35	0.4079 (3)	−0.0055 (3)	0.7892 (2)	0.0232 (10)
H35	0.3535	−0.0601	0.7599	0.028*
C36	0.5205 (3)	0.0337 (3)	0.7730 (2)	0.0266 (11)
H36	0.5432	0.0056	0.7322	0.032*
C37	0.5987 (4)	0.1132 (3)	0.8160 (2)	0.0293 (11)
H37	0.6753	0.1391	0.8047	0.035*
C38	0.5674 (3)	0.1552 (3)	0.8750 (2)	0.0298 (11)
H38	0.6215	0.2102	0.9041	0.036*
C39	0.4555 (3)	0.1166 (3)	0.8918 (2)	0.0248 (10)
H39	0.4332	0.1449	0.9326	0.030*
C40	0.2337 (3)	0.0481 (3)	0.9670 (2)	0.0191 (9)
C41	0.1825 (3)	0.1263 (3)	0.9782 (2)	0.0258 (10)
H41	0.1364	0.1451	0.9402	0.031*
C42	0.1997 (4)	0.1764 (3)	1.0452 (2)	0.0332 (11)
H42	0.1635	0.2290	1.0535	0.040*
C43	0.2689 (4)	0.1504 (3)	1.1000 (2)	0.0316 (11)
H43	0.2822	0.1859	1.1458	0.038*
C44	0.3193 (4)	0.0720 (3)	1.0878 (3)	0.0341 (12)
H44	0.3669	0.0539	1.1256	0.041*
C45	0.3010 (3)	0.0211 (3)	1.0224 (2)	0.0260 (10)
H45	0.3344	−0.0331	1.0146	0.031*
C46	0.2145 (3)	−0.1450 (3)	0.8706 (2)	0.0185 (9)
C47	0.1008 (4)	−0.2095 (3)	0.8511 (2)	0.0259 (10)
H47	0.0264	−0.1890	0.8384	0.031*
C48	0.0965 (4)	−0.3036 (3)	0.8503 (2)	0.0339 (11)
H48	0.0189	−0.3480	0.8361	0.041*
C49	0.2026 (4)	−0.3335 (3)	0.8697 (2)	0.0351 (12)
H49	0.1983	−0.3985	0.8690	0.042*
C50	0.3170 (4)	−0.2694 (3)	0.8905 (2)	0.0363 (12)
H50	0.3906	−0.2906	0.9039	0.044*
C51	0.3234 (4)	−0.1752 (3)	0.8916 (2)	0.0291 (11)
H51	0.4010	−0.1310	0.9065	0.035*
C52	0.0856 (3)	0.0065 (3)	0.8148 (2)	0.0194 (9)
C53	0.0986 (3)	0.0386 (3)	0.7547 (2)	0.0227 (10)
H53	0.1779	0.0509	0.7430	0.027*
C54	−0.0039 (4)	0.0532 (3)	0.7110 (2)	0.0304 (11)
H54	0.0049	0.0753	0.6695	0.037*
C55	−0.1190 (4)	0.0349 (3)	0.7289 (2)	0.0341 (12)
H55	−0.1895	0.0445	0.6993	0.041*
C56	−0.1322 (4)	0.0031 (3)	0.7889 (2)	0.0349 (12)
H56	−0.2116	−0.0094	0.8005	0.042*
C57	−0.0297 (3)	−0.0110 (3)	0.8329 (2)	0.0274 (11)
H57	−0.0384	−0.0324	0.8747	0.033*
O1	0.7306 (3)	0.7250 (3)	0.11497 (19)	0.0523 (10)

C58	0.6757 (5)	0.6490 (4)	0.0771 (3)	0.0495 (14)
C59	0.5588 (4)	0.6405 (3)	0.0192 (2)	0.0462 (13)
H59A	0.4876	0.5977	0.0282	0.069*
H59B	0.5749	0.6158	−0.0261	0.069*
H59C	0.5405	0.7027	0.0192	0.069*
C60	0.7210 (4)	0.5618 (3)	0.0854 (3)	0.0519 (14)
H60A	0.8022	0.5789	0.1174	0.078*
H60B	0.7288	0.5294	0.0401	0.078*
H60C	0.6617	0.5202	0.1041	0.078*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01975 (15)	0.01821 (17)	0.02061 (19)	0.00369 (11)	0.00614 (12)	0.00437 (14)
S1	0.0259 (6)	0.0219 (6)	0.0309 (8)	0.0022 (4)	0.0099 (5)	0.0084 (5)
S2	0.0271 (6)	0.0254 (6)	0.0262 (7)	0.0110 (5)	0.0115 (5)	0.0112 (5)
C1	0.033 (2)	0.013 (2)	0.018 (3)	0.0033 (17)	0.0047 (19)	0.005 (2)
C2	0.024 (2)	0.024 (3)	0.019 (3)	0.0057 (18)	0.0017 (19)	0.006 (2)
S3	0.0357 (6)	0.0265 (7)	0.0264 (8)	−0.0010 (5)	0.0032 (5)	0.0103 (6)
S4	0.0285 (6)	0.0243 (7)	0.0312 (8)	0.0063 (5)	0.0006 (5)	0.0104 (6)
C3	0.034 (2)	0.010 (2)	0.028 (3)	−0.0072 (17)	−0.003 (2)	0.001 (2)
S5	0.0419 (7)	0.0257 (7)	0.0405 (9)	−0.0021 (5)	−0.0117 (6)	0.0157 (6)
S6	0.0314 (6)	0.0212 (6)	0.0238 (7)	0.0082 (5)	0.0033 (5)	0.0018 (5)
S7	0.0244 (6)	0.0264 (7)	0.0277 (7)	0.0074 (5)	0.0092 (5)	0.0042 (5)
C4	0.019 (2)	0.023 (3)	0.026 (3)	0.0050 (17)	−0.0032 (19)	0.004 (2)
C5	0.015 (2)	0.019 (2)	0.032 (3)	0.0049 (17)	0.0027 (19)	−0.002 (2)
S8	0.0322 (6)	0.0283 (7)	0.0269 (7)	0.0097 (5)	0.0035 (5)	0.0081 (6)
S9	0.0274 (6)	0.0271 (7)	0.0344 (8)	0.0099 (5)	0.0096 (5)	0.0068 (6)
C6	0.017 (2)	0.022 (3)	0.047 (3)	0.0078 (17)	0.008 (2)	0.012 (2)
S10	0.0386 (7)	0.0337 (7)	0.0411 (9)	0.0150 (5)	0.0075 (6)	0.0138 (6)
S11	0.0258 (6)	0.0226 (6)	0.0198 (7)	0.0004 (4)	0.0042 (5)	0.0080 (5)
S12	0.0249 (6)	0.0222 (6)	0.0211 (7)	0.0006 (4)	0.0031 (5)	0.0081 (5)
C7	0.019 (2)	0.018 (2)	0.020 (3)	0.0025 (16)	0.0027 (18)	0.003 (2)
C8	0.017 (2)	0.018 (2)	0.027 (3)	0.0047 (16)	0.0049 (18)	0.007 (2)
S13	0.0283 (6)	0.0239 (6)	0.0236 (7)	0.0017 (5)	0.0035 (5)	0.0057 (5)
S14	0.0218 (5)	0.0203 (6)	0.0251 (7)	0.0023 (4)	0.0052 (5)	0.0068 (5)
C9	0.020 (2)	0.024 (2)	0.024 (3)	0.0067 (17)	0.0081 (18)	0.007 (2)
S15	0.0340 (6)	0.0256 (7)	0.0346 (8)	−0.0028 (5)	0.0049 (5)	0.0020 (6)
As1	0.0175 (2)	0.0167 (2)	0.0183 (3)	0.00286 (16)	0.00455 (18)	0.0034 (2)
C10	0.020 (2)	0.016 (2)	0.014 (2)	0.0032 (16)	0.0066 (18)	0.0049 (19)
C11	0.018 (2)	0.025 (3)	0.020 (3)	0.0017 (18)	0.0074 (18)	0.006 (2)
C12	0.030 (2)	0.017 (2)	0.032 (3)	0.0066 (19)	0.017 (2)	0.008 (2)
C13	0.028 (2)	0.022 (3)	0.039 (3)	0.0116 (19)	0.018 (2)	0.020 (2)
C14	0.016 (2)	0.036 (3)	0.023 (3)	0.0083 (19)	0.0040 (18)	0.013 (2)
C15	0.021 (2)	0.024 (2)	0.017 (3)	0.0052 (18)	0.0055 (18)	0.000 (2)
C16	0.016 (2)	0.016 (2)	0.022 (3)	0.0038 (16)	0.0063 (18)	0.004 (2)
C17	0.026 (2)	0.022 (3)	0.019 (3)	0.0014 (18)	0.0073 (19)	0.005 (2)
C18	0.034 (3)	0.015 (2)	0.027 (3)	0.0006 (19)	−0.001 (2)	0.002 (2)

C19	0.021 (2)	0.027 (3)	0.026 (3)	−0.0012 (18)	0.0038 (19)	0.014 (2)
C20	0.022 (2)	0.032 (3)	0.034 (3)	0.0091 (19)	0.013 (2)	0.013 (2)
C21	0.023 (2)	0.023 (2)	0.021 (3)	0.0041 (18)	0.0095 (19)	0.004 (2)
C22	0.018 (2)	0.018 (2)	0.018 (3)	−0.0025 (17)	0.0092 (18)	0.002 (2)
C23	0.032 (2)	0.020 (2)	0.022 (3)	0.0061 (19)	0.010 (2)	0.005 (2)
C24	0.034 (3)	0.024 (3)	0.037 (3)	0.004 (2)	0.013 (2)	0.001 (2)
C25	0.035 (3)	0.023 (3)	0.034 (3)	−0.006 (2)	0.017 (2)	−0.003 (2)
C26	0.033 (3)	0.035 (3)	0.019 (3)	−0.002 (2)	0.006 (2)	0.003 (2)
C27	0.019 (2)	0.023 (2)	0.022 (3)	−0.0010 (17)	0.0049 (19)	0.004 (2)
C28	0.0114 (19)	0.021 (2)	0.014 (2)	0.0046 (16)	0.0007 (16)	−0.0021 (19)
C29	0.017 (2)	0.024 (2)	0.023 (3)	0.0098 (17)	0.0051 (19)	0.004 (2)
C30	0.025 (2)	0.038 (3)	0.022 (3)	0.015 (2)	0.009 (2)	0.008 (2)
C31	0.015 (2)	0.040 (3)	0.023 (3)	0.0054 (19)	−0.0006 (19)	−0.006 (2)
C32	0.019 (2)	0.027 (3)	0.027 (3)	0.0020 (18)	0.010 (2)	0.002 (2)
C33	0.022 (2)	0.025 (3)	0.022 (3)	0.0063 (18)	0.0043 (19)	0.004 (2)
As2	0.0164 (2)	0.0180 (2)	0.0227 (3)	0.00394 (16)	0.00378 (18)	0.0039 (2)
C34	0.015 (2)	0.017 (2)	0.031 (3)	0.0055 (17)	0.0035 (19)	0.010 (2)
C35	0.022 (2)	0.020 (2)	0.029 (3)	0.0083 (18)	0.0018 (19)	0.008 (2)
C36	0.025 (2)	0.026 (3)	0.035 (3)	0.0099 (19)	0.012 (2)	0.014 (2)
C37	0.021 (2)	0.028 (3)	0.045 (3)	0.008 (2)	0.009 (2)	0.022 (3)
C38	0.018 (2)	0.024 (3)	0.043 (3)	−0.0007 (18)	0.001 (2)	0.008 (2)
C39	0.024 (2)	0.023 (3)	0.027 (3)	0.0080 (18)	0.005 (2)	0.000 (2)
C40	0.016 (2)	0.019 (2)	0.019 (3)	−0.0014 (17)	0.0023 (18)	0.002 (2)
C41	0.032 (2)	0.022 (3)	0.023 (3)	0.0106 (19)	0.002 (2)	0.002 (2)
C42	0.039 (3)	0.023 (3)	0.036 (3)	0.011 (2)	0.008 (2)	−0.003 (2)
C43	0.032 (3)	0.034 (3)	0.020 (3)	−0.004 (2)	0.004 (2)	−0.007 (2)
C44	0.027 (2)	0.042 (3)	0.032 (3)	0.004 (2)	0.003 (2)	0.013 (3)
C45	0.031 (2)	0.027 (3)	0.023 (3)	0.0113 (19)	0.008 (2)	0.007 (2)
C46	0.025 (2)	0.016 (2)	0.018 (3)	0.0069 (17)	0.0092 (18)	0.0044 (19)
C47	0.033 (2)	0.027 (3)	0.018 (3)	0.0057 (19)	0.004 (2)	0.006 (2)
C48	0.045 (3)	0.024 (3)	0.026 (3)	−0.006 (2)	0.005 (2)	0.004 (2)
C49	0.059 (3)	0.021 (3)	0.031 (3)	0.011 (2)	0.020 (3)	0.009 (2)
C50	0.048 (3)	0.037 (3)	0.038 (3)	0.026 (2)	0.022 (2)	0.016 (3)
C51	0.025 (2)	0.027 (3)	0.039 (3)	0.0106 (19)	0.012 (2)	0.008 (2)
C52	0.017 (2)	0.016 (2)	0.024 (3)	0.0047 (16)	0.0019 (18)	0.003 (2)
C53	0.020 (2)	0.021 (2)	0.029 (3)	0.0047 (17)	0.0068 (19)	0.009 (2)
C54	0.042 (3)	0.019 (3)	0.032 (3)	0.012 (2)	0.006 (2)	0.008 (2)
C55	0.027 (3)	0.043 (3)	0.031 (3)	0.018 (2)	−0.003 (2)	0.005 (3)
C56	0.023 (2)	0.054 (3)	0.032 (3)	0.016 (2)	0.009 (2)	0.012 (3)
C57	0.026 (2)	0.040 (3)	0.020 (3)	0.013 (2)	0.005 (2)	0.008 (2)
O1	0.057 (2)	0.049 (3)	0.047 (3)	0.0056 (18)	0.0026 (19)	0.016 (2)
C58	0.075 (4)	0.054 (4)	0.032 (4)	0.025 (3)	0.024 (3)	0.020 (3)
C59	0.072 (4)	0.039 (3)	0.024 (3)	0.015 (3)	0.008 (3)	−0.005 (3)
C60	0.076 (4)	0.062 (4)	0.023 (3)	0.031 (3)	0.008 (3)	0.010 (3)

Geometric parameters (Å, º)

Sn1—S12	2.5310 (10)	C28—C29	1.392 (5)
Sn1—S11	2.5320 (11)	C29—C30	1.384 (5)
Sn1—S1	2.5503 (10)	C29—H29	0.9500
Sn1—S7	2.5517 (10)	C30—C31	1.383 (5)
Sn1—S2	2.5553 (10)	C30—H30	0.9500
Sn1—S6	2.5585 (12)	C31—C32	1.376 (5)
S1—C1	1.734 (4)	C31—H31	0.9500
S2—C2	1.732 (4)	C32—C33	1.379 (5)
C1—C2	1.369 (5)	C32—H32	0.9500
C1—S3	1.746 (4)	C33—H33	0.9500
C2—S4	1.750 (4)	As2—C40	1.901 (4)
S3—C3	1.739 (4)	As2—C52	1.903 (4)
S4—C3	1.722 (4)	As2—C46	1.905 (4)
C3—S5	1.651 (4)	As2—C34	1.913 (3)
S6—C4	1.752 (4)	C34—C39	1.382 (5)
S7—C5	1.729 (4)	C34—C35	1.386 (5)
C4—C5	1.349 (5)	C35—C36	1.397 (5)
C4—S8	1.749 (4)	C35—H35	0.9500
C5—S9	1.759 (4)	C36—C37	1.382 (6)
S8—C6	1.715 (4)	C36—H36	0.9500
S9—C6	1.760 (4)	C37—C38	1.376 (6)
C6—S10	1.642 (4)	C37—H37	0.9500
S11—C7	1.749 (4)	C38—C39	1.393 (5)
S12—C8	1.737 (4)	C38—H38	0.9500
C7—C8	1.363 (5)	C39—H39	0.9500
C7—S13	1.740 (4)	C40—C45	1.384 (5)
C8—S14	1.748 (4)	C40—C41	1.392 (5)
S13—C9	1.726 (4)	C41—C42	1.383 (6)
S14—C9	1.718 (4)	C41—H41	0.9500
C9—S15	1.662 (4)	C42—C43	1.378 (6)
As1—C28	1.901 (4)	C42—H42	0.9500
As1—C10	1.908 (3)	C43—C44	1.391 (5)
As1—C22	1.910 (4)	C43—H43	0.9500
As1—C16	1.912 (3)	C44—C45	1.360 (6)
C10—C11	1.383 (5)	C44—H44	0.9500
C10—C15	1.393 (5)	C45—H45	0.9500
C11—C12	1.394 (5)	C46—C47	1.388 (5)
C11—H11	0.9500	C46—C51	1.400 (5)
C12—C13	1.382 (5)	C47—C48	1.379 (5)
C12—H12	0.9500	C47—H47	0.9500
C13—C14	1.383 (5)	C48—C49	1.365 (5)
C13—H13	0.9500	C48—H48	0.9500
C14—C15	1.374 (5)	C49—C50	1.392 (6)
C14—H14	0.9500	C49—H49	0.9500
C15—H15	0.9500	C50—C51	1.377 (5)
C16—C17	1.387 (5)	C50—H50	0.9500

C16—C21	1.389 (5)	C51—H51	0.9500
C17—C18	1.390 (5)	C52—C53	1.376 (5)
C17—H17	0.9500	C52—C57	1.390 (5)
C18—C19	1.381 (5)	C53—C54	1.392 (5)
C18—H18	0.9500	C53—H53	0.9500
C19—C20	1.367 (5)	C54—C55	1.387 (5)
C19—H19	0.9500	C54—H54	0.9500
C20—C21	1.376 (5)	C55—C56	1.374 (6)
C20—H20	0.9500	C55—H55	0.9500
C21—H21	0.9500	C56—C57	1.391 (5)
C22—C27	1.384 (5)	C56—H56	0.9500
C22—C23	1.390 (5)	C57—H57	0.9500
C23—C24	1.386 (5)	O1—C58	1.230 (6)
C23—H23	0.9500	C58—C60	1.496 (6)
C24—C25	1.380 (6)	C58—C59	1.561 (7)
C24—H24	0.9500	C59—H59A	0.9800
C25—C26	1.379 (5)	C59—H59B	0.9800
C25—H25	0.9500	C59—H59C	0.9800
C26—C27	1.388 (5)	C60—H60A	0.9800
C26—H26	0.9500	C60—H60B	0.9800
C27—H27	0.9500	C60—H60C	0.9800
C28—C33	1.388 (5)		

S12—Sn1—S11	87.42 (3)	C26—C27—H27	120.1
S12—Sn1—S1	173.46 (3)	C33—C28—C29	120.8 (4)
S11—Sn1—S1	89.51 (3)	C33—C28—As1	119.4 (3)
S12—Sn1—S7	96.99 (3)	C29—C28—As1	119.8 (3)
S11—Sn1—S7	93.20 (4)	C30—C29—C28	119.3 (4)
S1—Sn1—S7	88.95 (3)	C30—C29—H29	120.4
S12—Sn1—S2	91.63 (3)	C28—C29—H29	120.4
S11—Sn1—S2	96.46 (3)	C31—C30—C29	119.9 (4)
S1—Sn1—S2	82.97 (3)	C31—C30—H30	120.1
S7—Sn1—S2	167.34 (4)	C29—C30—H30	120.1
S12—Sn1—S6	86.64 (3)	C32—C31—C30	120.5 (4)
S11—Sn1—S6	171.55 (3)	C32—C31—H31	119.8
S1—Sn1—S6	97.00 (4)	C30—C31—H31	119.8
S7—Sn1—S6	81.59 (3)	C31—C32—C33	120.6 (4)
S2—Sn1—S6	89.70 (3)	C31—C32—H32	119.7
C1—S1—Sn1	96.10 (12)	C33—C32—H32	119.7
C2—S2—Sn1	96.31 (13)	C32—C33—C28	119.0 (4)
C2—C1—S1	125.5 (3)	C32—C33—H33	120.5
C2—C1—S3	115.5 (3)	C28—C33—H33	120.5
S1—C1—S3	119.1 (2)	C40—As2—C52	109.20 (16)
C1—C2—S2	125.5 (3)	C40—As2—C46	110.43 (16)
C1—C2—S4	115.4 (3)	C52—As2—C46	110.84 (16)
S2—C2—S4	119.1 (2)	C40—As2—C34	107.38 (17)
C3—S3—C1	98.40 (18)	C52—As2—C34	111.38 (16)
C3—S4—C2	98.65 (18)	C46—As2—C34	107.55 (15)

S5—C3—S4	124.1 (2)	C39—C34—C35	121.0 (4)
S5—C3—S3	123.8 (2)	C39—C34—As2	118.2 (3)
S4—C3—S3	112.1 (2)	C35—C34—As2	120.7 (3)
C4—S6—Sn1	92.15 (14)	C34—C35—C36	118.7 (4)
C5—S7—Sn1	92.63 (12)	C34—C35—H35	120.6
C5—C4—S8	116.7 (3)	C36—C35—H35	120.6
C5—C4—S6	124.5 (3)	C37—C36—C35	120.1 (4)
S8—C4—S6	118.2 (2)	C37—C36—H36	119.9
C4—C5—S7	125.3 (3)	C35—C36—H36	119.9
C4—C5—S9	115.0 (3)	C38—C37—C36	120.9 (4)
S7—C5—S9	118.9 (2)	C38—C37—H37	119.5
C6—S8—C4	98.5 (2)	C36—C37—H37	119.5
C5—S9—C6	97.98 (19)	C37—C38—C39	119.4 (4)
S10—C6—S8	125.6 (3)	C37—C38—H38	120.3
S10—C6—S9	122.6 (2)	C39—C38—H38	120.3
S8—C6—S9	111.8 (2)	C34—C39—C38	119.8 (4)
C7—S11—Sn1	98.47 (14)	C34—C39—H39	120.1
C8—S12—Sn1	98.54 (13)	C38—C39—H39	120.1
C8—C7—S13	115.8 (3)	C45—C40—C41	120.3 (4)
C8—C7—S11	127.4 (3)	C45—C40—As2	119.8 (3)
S13—C7—S11	116.8 (2)	C41—C40—As2	119.6 (3)
C7—C8—S12	128.1 (3)	C42—C41—C40	119.1 (4)
C7—C8—S14	115.0 (3)	C42—C41—H41	120.4
S12—C8—S14	116.9 (2)	C40—C41—H41	120.4
C9—S13—C7	98.37 (19)	C43—C42—C41	120.4 (4)
C9—S14—C8	98.65 (19)	C43—C42—H42	119.8
S15—C9—S14	124.1 (2)	C41—C42—H42	119.8
S15—C9—S13	123.7 (3)	C42—C43—C44	119.6 (4)
S14—C9—S13	112.2 (2)	C42—C43—H43	120.2
C28—As1—C10	110.72 (16)	C44—C43—H43	120.2
C28—As1—C22	108.08 (15)	C45—C44—C43	120.5 (4)
C10—As1—C22	110.95 (16)	C45—C44—H44	119.7
C28—As1—C16	109.94 (16)	C43—C44—H44	119.7
C10—As1—C16	108.01 (14)	C44—C45—C40	120.0 (4)
C22—As1—C16	109.13 (16)	C44—C45—H45	120.0
C11—C10—C15	120.6 (3)	C40—C45—H45	120.0
C11—C10—As1	121.3 (3)	C47—C46—C51	120.0 (4)
C15—C10—As1	118.2 (3)	C47—C46—As2	121.3 (3)
C10—C11—C12	118.9 (4)	C51—C46—As2	118.6 (3)
C10—C11—H11	120.5	C48—C47—C46	119.6 (4)
C12—C11—H11	120.5	C48—C47—H47	120.2
C13—C12—C11	120.5 (4)	C46—C47—H47	120.2
C13—C12—H12	119.8	C49—C48—C47	120.6 (4)
C11—C12—H12	119.8	C49—C48—H48	119.7
C12—C13—C14	120.0 (4)	C47—C48—H48	119.7
C12—C13—H13	120.0	C48—C49—C50	120.4 (4)
C14—C13—H13	120.0	C48—C49—H49	119.8
C15—C14—C13	120.2 (4)	C50—C49—H49	119.8

C15—C14—H14	119.9	C51—C50—C49	119.9 (4)
C13—C14—H14	119.9	C51—C50—H50	120.0
C14—C15—C10	119.8 (4)	C49—C50—H50	120.0
C14—C15—H15	120.1	C50—C51—C46	119.5 (4)
C10—C15—H15	120.1	C50—C51—H51	120.3
C17—C16—C21	121.5 (3)	C46—C51—H51	120.3
C17—C16—As1	120.6 (3)	C53—C52—C57	120.4 (3)
C21—C16—As1	117.9 (3)	C53—C52—As2	120.6 (3)
C16—C17—C18	118.6 (4)	C57—C52—As2	119.0 (3)
C16—C17—H17	120.7	C52—C53—C54	120.4 (3)
C18—C17—H17	120.7	C52—C53—H53	119.8
C19—C18—C17	119.9 (4)	C54—C53—H53	119.8
C19—C18—H18	120.1	C55—C54—C53	119.0 (4)
C17—C18—H18	120.1	C55—C54—H54	120.5
C20—C19—C18	120.5 (4)	C53—C54—H54	120.5
C20—C19—H19	119.7	C56—C55—C54	120.7 (4)
C18—C19—H19	119.7	C56—C55—H55	119.6
C19—C20—C21	121.0 (4)	C54—C55—H55	119.6
C19—C20—H20	119.5	C55—C56—C57	120.3 (4)
C21—C20—H20	119.5	C55—C56—H56	119.9
C20—C21—C16	118.4 (4)	C57—C56—H56	119.9
C20—C21—H21	120.8	C52—C57—C56	119.2 (4)
C16—C21—H21	120.8	C52—C57—H57	120.4
C27—C22—C23	120.5 (4)	C56—C57—H57	120.4
C27—C22—As1	122.1 (3)	O1—C58—C60	120.2 (5)
C23—C22—As1	117.3 (3)	O1—C58—C59	121.6 (4)
C24—C23—C22	119.5 (4)	C60—C58—C59	118.2 (5)
C24—C23—H23	120.3	C58—C59—H59A	109.5
C22—C23—H23	120.3	C58—C59—H59B	109.5
C25—C24—C23	119.7 (4)	H59A—C59—H59B	109.5
C25—C24—H24	120.2	C58—C59—H59C	109.5
C23—C24—H24	120.2	H59A—C59—H59C	109.5
C26—C25—C24	121.1 (4)	H59B—C59—H59C	109.5
C26—C25—H25	119.5	C58—C60—H60A	109.5
C24—C25—H25	119.5	C58—C60—H60B	109.5
C25—C26—C27	119.4 (4)	H60A—C60—H60B	109.5
C25—C26—H26	120.3	C58—C60—H60C	109.5
C27—C26—H26	120.3	H60A—C60—H60C	109.5
C22—C27—C26	119.8 (4)	H60B—C60—H60C	109.5
C22—C27—H27	120.1		