Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

9-Sila-9,9″-spirobixanthene

Joel T. Mague,[a]* Maravanji S. Balakrishna[b] and Ramalingam Venkateswaran[b]

[a]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA, and [b]Department of Chemistry, Indian Institute of Technology Bombay, Mumbai 400 076, India
Correspondence e-mail: joelt@tulane.edu

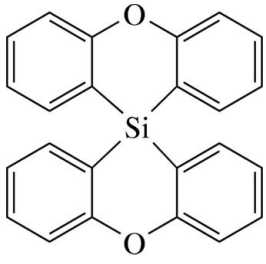
Received 17 October 2007; accepted 18 October 2007

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.098; data-to-parameter ratio = 18.4.

The title molecule, $C_{24}H_{16}O_2Si$, exhibits slightly distorted tetrahedral coordination about silicon, a slight folding of each half of the molecule about the Si···O line, and π–π and C—H···π-ring interactions.

Related literature

For related literature, see: Armaroli *et al.* (2006); Hitchcock *et al.* (1957); Kuwano *et al.* (2003); Noyori (2002); Oita & Gilman (1957); Zhang *et al.* (2006); Kranenburg *et al.* (1995).



Experimental

Crystal data

$C_{24}H_{16}O_2Si$
M_r = 364.46
Monoclinic, $P2_1/c$
a = 10.7975 (7) Å
b = 11.4290 (7) Å
c = 14.0515 (9) Å
β = 92.756 (1)°
V = 1732.0 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 100 (2) K
0.28 × 0.12 × 0.12 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2007)
T_{min} = 0.881, T_{max} = 0.982
31348 measured reflections
4517 independent reflections
3962 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.098
S = 1.04
4517 reflections
245 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Si1—C12	1.847 (1)	Si1—C1	1.852 (1)
Si1—C13	1.850 (1)	Si1—C24	1.857 (1)
C12—Si1—C13	115.69 (6)	C12—Si1—C24	111.85 (5)
C12—Si1—C1	100.57 (6)	C13—Si1—C24	100.31 (6)
C13—Si1—C1	114.41 (5)	C1—Si1—C24	114.70 (5)

Table 2
Interplanar angles (°).

Plane[a]	Plane	Dihedral angle
1	2	86.14 (3)
3	4	5.66 (4)
5	6	9.30 (5)
7	8	6.54 (6)

Note: (*a*) atoms defining planes: (1) Si1/O1/C1/C6/C7/C12; (2) Si1/O2/C13/C18/C19/C24; (3) Si1/O1/C1–C6; (4) Si1/O1/C7–C12; (5) Si1/O2/C13–C18; (6) Si1/O2/C19–C24; (7) C1–C6; (8) C7–C12 at $(2-x, 1-y, -z)$.

Table 3
Intermolecular contacts (Å).

Contact	Distance
$Cg(7)\cdots Cg(8)^{a,b}$	3.96
$d(8\cdots 9)^{c}$	3.34
C15—H15$\cdots Cg(9)$	2.68

Notes: (*a*) atoms defining planes: (7) C1–C6; (8) C7–C12 at $(2-x, 1-y, -z)$; (9) C1–C6 at $(x, \frac{3}{2}+y, -\frac{1}{2}+z)$; (*b*) *Cg* = center of gravity of specified ring; (*c*) perpendicular distance between specified rings.

Data collection: *CELL_NOW* (Sheldrick, 2005) and *APEX2* (Bruker, 2007); cell refinement: *APEX2*; data reduction: *SAINT-Plus* (Bruker, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *APEX2*; software used to prepare material for publication: *APEX2*.

The authors thank the Chemistry Department of Tulane University for use of the X-ray laboratory and the Louisiana Educational Quality Support Fund, administered by the Louisiana Board of Regents, for purchase of the CCD diffractometer under grant No. LEQSF (2002–03)-ENH-TR-67.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SK3175).

References

Armaroli, N., Accorsi, G., Holler, M., Moudam, O., Nierengarten, J.-F., Zhou, Z., Wegh, R. T. & Welter, R. (2006). *Adv. Mater.* **18**, 1313–1316.
Bruker (2006). *SAINT-Plus*. Version 7.34A. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *APEX2*. Version 2.1-4. Bruker AXS Inc., Madison, Wisconsin, USA.
Hitchcock, C. H. S., Mann, F. G. & Vanterpool, A. (1957). *J. Chem. Soc.* pp. 4537–4546.

Kranenburg, M., van der Burgt, Y. E. M., Kamer, P. C. J., van Leeuwen, P. W. N. M., Goubitz, K. & Fraanje, J. (1995). *Organometallics*, **14**, 3081–3089.
Kuwano, R., Kondo, Y. & Matsuyama, Y. (2003). *J. Am. Chem. Soc.* **125**, 12104–12105.
Noyori, R. (2002). *Angew. Chem. Int. Ed.* **41**, 2008–2022.
Oita, K. & Gilman, H. (1957). *J. Am. Chem. Soc.* **79**, 339–342.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2005). *CELL_NOW*. University of Göttingen, Germany.
Sheldrick, G. M. (2007). *TWINABS*. Version 2007/5. University of Göttingen, Germany.
Zhang, Q., Zhou, Q., Cheng, Y., Wang, L., Ma, D., Jing, X. & Wang, F. (2006). *Adv. Funct. Mater.* **16**, 1203–1208.

supplementary materials

Acta Cryst. (2007). E**63**, o4429-o4430 [**doi:10.1107/S1600536807051604**]

9-Sila-9,9''-spirobixanthene

J. T. Mague, M. S. Balakrishna and R. Venkateswaran

Comment

The syntheses of diphenylether derivatives such as 2,2'-dilithiodiphenylether (I), 10,10'-diphenylphenoxasilane (II), 10-diphenylphenoxyphosphine (III) and 10,10'-spirobi(dibenzo[b,e][1,4]oxa)silane (IV) were first reported by Hitchcock *et al.* (1957) and Oita & Gilman (1957). Subsequently, some of these derivatives were used extensively to make interesting phosphorus(III) based ligands for coordination chemistry (Noyori, 2002), luminescence (Armaroli *et al.*, 2006) and sensor materials (Zhang *et al.*, 2006), organic light emitting devices and catalytic applications (Kranenburg *et al.*, 1995) (Kuwano *et al.*, 2003). Despite the wide interest in this class of compounds, structural data are not available for the spirocyclic derivative IV.

A perspective view of IV is presented in Figure 1. The geometry about silicon is slightly distorted tetrahedral as can be seen from the data in Table 1 and the dihedral angle of 86.14 (3)° between the Si1 O1 C1 C6 C7 C12 and Si1 O2 C13 C18 C19 C24 planes. Each 1-Si,2-O—C_6H_4 moiety is within 0.04 Å of planarity but in the half of the molecule containing C1—C12, Si1 and O1, the two 1-Si,2-O—C_6H_4 moieties are folded about the Si1—O1 line by 5.66 (4)° while in the other half of the molecule the fold angle is 9.30 (5)°. Assisting in assembling the crystal structure are π-π and C—H–π-ring interactions. The first occurs between the C1—C6 ring and the C7—C12 ring in the molecule at 2 − *x*, 1 − *y*, −*z* where the dihedral angle between the planes is 6.54°, the distance between the centers of gravity (*Cg*) of the rings is 3.6907 (7) Å and the average perpendicular distance between the rings is 3.34 Å. The second occrs between C15—H15 and the ring consisting of C1—C6 at *x*, 1.5 − *y*, −1/2 + *z* where the distance from H15 to the center of gravity of the ring is 2.68 Å and the C—H–*Cg* angle is 148°.

Experimental

The title compound was prepared by a modification of the published method (Oita & Gilman, 1957). A solution of diphenyl ether (8 ml, 50.3 mmol) in THF (50 ml) was added dropwise to a mixture of n-BuLi (92.3 ml, 110 mmol, 1.6 *M* in hexanes) and TMEDA (16.7 ml, 110 mmol) and the mixture was stirred for 12 h. A solution of silicon tetrachloride (2.9 ml, 50.3 mmol) in THF (30 ml) was added and stirring was continued for a further period of 16 h. To the stirred solution 20 ml of water was added and the organic layer was separated. After extracting the aqueous layer twice with diethyl ether, the combined organic layers were treated with activated charcoal and dried with anhydrous $MgSO_4$. The solvent was removed *in vacuo* to obtain a yellow solid which was purified by chromatography and recrystallized from a 1:2 mixture of dichloromethane and petroleum ether. Yield: 3.5 g (39%). Mp: >523 K. Anal. Calcd for $C_{24}H_{16}SiO_2$: C,79.09; H, 4.43%. Found: C, 78.73; H, 3.95%. MS, EI (m/*z*): 364.5 (*M*+). ^{1}H NMR ($CDCl_3$): δ 6.95–7.50 (m, phenyl).

Refinement

From 1170 reflections harvested from diverse regions of reciprocal space and having I/σ(I) > 15 it was determined (CELL_NOW (Sheldrick, 2005)) that the compound crystallized in the monoclinic system and that the crystal was twinned

by a 177.4° rotation about the *b* axis. Integration of the raw data was performed with the 2-component version of *SAINT+* as controlled by the 2-component instruction file generated by CELL_NOW. Correction for absorption and crystal decay as well as deconvolution of the overlapped reflections was performed with TWINABS (Sheldrick, 2007) which also generated a reflection file containing only the single reflections from the major component which was used for the solution and preliminary refinement of the structure. Final refinement was carried out with a reflection file containing all single reflections from the major twin component plus that portion of all composite reflections attibutable to that component. The twin fraction is 0.31

Figures

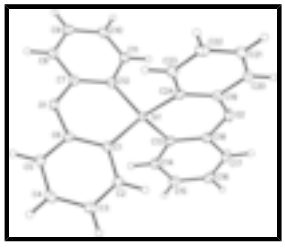


Fig. 1. Perspective view of IV. Displacement ellipsoids are drawn at the 50% level and H-atoms are represented by spheres of arbitrary radius.

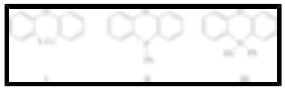


Fig. 2. The structures of (I), (II) and (III).

9-Sila-9,9''-spirobixanthene

Crystal data

$C_{24}H_{16}O_2Si$	F_{000} = 760
M_r = 364.46	D_x = 1.398 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4009 reflections
a = 10.7975 (7) Å	θ = 2.6–29.1º
b = 11.4290 (7) Å	μ = 0.15 mm^{-1}
c = 14.0515 (9) Å	T = 100 (2) K
β = 92.756 (1)º	Block, colourless
V = 1732.0 (2) Å^3	0.28 × 0.12 × 0.12 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	4517 independent reflections
Radiation source: fine-focus sealed tube	3962 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.038
T = 100(2) K	θ_{max} = 28.9º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (TWINABS; Sheldrick, 2007)	h = −14→14

T_{min} = 0.881, T_{max} = 0.982	k = −15→15
31348 measured reflections	l = −19→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.037	H-atom parameters constrained
$wR(F^2)$ = 0.098	$w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 0.6911P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
4517 reflections	$\Delta\rho_{max}$ = 0.42 e Å^{-3}
245 parameters	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5 °. in omega, colllected at phi = 0.00, 90.00 and 180.00 °. and 2 sets of 800 frames, each of width 0.45 ° in phi, collected at omega = −30.00 and 210.00 °. The scan time was 20 sec/frame.

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. H-atoms were placed in calculated positions (C—H = 0.95 Å) and included as riding contributions with isotropic displacement parameters 1.2 times those of the attached carbon atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Si1	0.79679 (3)	0.68709 (3)	0.09949 (2)	0.01172 (9)
O1	0.93646 (8)	0.44025 (8)	0.10359 (6)	0.01635 (19)
O2	0.61910 (9)	0.91110 (8)	0.09843 (7)	0.0195 (2)
C1	0.94750 (11)	0.64573 (11)	0.15843 (8)	0.0131 (2)
C2	1.02066 (11)	0.72674 (11)	0.21191 (9)	0.0151 (2)
H2	0.9918	0.8048	0.2175	0.018*
C3	1.13318 (12)	0.69630 (11)	0.25648 (9)	0.0170 (2)
H3	1.1798	0.7524	0.2929	0.020*
C4	1.17750 (11)	0.58234 (12)	0.24735 (9)	0.0166 (2)
H4	1.2549	0.5609	0.2774	0.020*
C5	1.10929 (11)	0.50053 (11)	0.19476 (9)	0.0147 (2)

H5	1.1400	0.4232	0.1880	0.018*
C6	0.99463 (11)	0.53219 (10)	0.15140 (8)	0.0128 (2)
C7	0.82770 (11)	0.44887 (11)	0.04799 (8)	0.0130 (2)
C8	0.79146 (11)	0.34298 (11)	0.00550 (9)	0.0150 (2)
H8	0.8387	0.2741	0.0179	0.018*
C9	0.68621 (12)	0.33901 (11)	−0.05482 (9)	0.0163 (2)
H9	0.6610	0.2670	−0.0835	0.020*
C10	0.61712 (12)	0.43994 (12)	−0.07369 (9)	0.0170 (2)
H10	0.5463	0.4377	−0.1164	0.020*
C11	0.65286 (11)	0.54342 (11)	−0.02949 (9)	0.0157 (2)
H11	0.6047	0.6118	−0.0420	0.019*
C12	0.75802 (11)	0.55123 (11)	0.03337 (8)	0.0134 (2)
C13	0.80137 (11)	0.82187 (10)	0.02678 (8)	0.0131 (2)
C14	0.89247 (11)	0.84005 (11)	−0.04049 (9)	0.0155 (2)
H14	0.9499	0.7792	−0.0516	0.019*
C15	0.90084 (12)	0.94368 (12)	−0.09083 (9)	0.0175 (2)
H15	0.9639	0.9539	−0.1350	0.021*
C16	0.81571 (12)	1.03291 (11)	−0.07603 (9)	0.0183 (3)
H16	0.8212	1.1045	−0.1099	0.022*
C17	0.72353 (12)	1.01763 (11)	−0.01233 (9)	0.0183 (3)
H17	0.6647	1.0779	−0.0032	0.022*
C18	0.71743 (11)	0.91282 (11)	0.03863 (9)	0.0145 (2)
C19	0.60334 (11)	0.82827 (11)	0.16857 (9)	0.0144 (2)
C20	0.50531 (12)	0.85513 (11)	0.22636 (9)	0.0174 (3)
H20	0.4576	0.9240	0.2149	0.021*
C21	0.47822 (12)	0.78099 (12)	0.30027 (9)	0.0182 (3)
H21	0.4115	0.7988	0.3395	0.022*
C22	0.54843 (12)	0.68018 (12)	0.31746 (9)	0.0183 (3)
H22	0.5306	0.6294	0.3686	0.022*
C23	0.64470 (11)	0.65506 (11)	0.25895 (9)	0.0160 (2)
H23	0.6923	0.5863	0.2711	0.019*
C24	0.67474 (11)	0.72721 (11)	0.18228 (8)	0.0132 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.01153 (16)	0.00995 (16)	0.01365 (17)	0.00109 (11)	0.00041 (12)	−0.00008 (11)
O1	0.0161 (4)	0.0115 (4)	0.0209 (4)	0.0018 (3)	−0.0052 (3)	−0.0014 (3)
O2	0.0205 (5)	0.0154 (4)	0.0235 (5)	0.0070 (4)	0.0088 (4)	0.0056 (4)
C1	0.0127 (5)	0.0137 (5)	0.0130 (5)	0.0008 (4)	0.0021 (4)	0.0013 (4)
C2	0.0160 (5)	0.0148 (6)	0.0148 (5)	−0.0004 (4)	0.0019 (4)	−0.0014 (4)
C3	0.0161 (6)	0.0199 (6)	0.0150 (6)	−0.0034 (5)	0.0000 (4)	−0.0012 (5)
C4	0.0125 (5)	0.0228 (6)	0.0144 (5)	0.0003 (5)	−0.0001 (4)	0.0034 (5)
C5	0.0145 (5)	0.0146 (6)	0.0151 (5)	0.0018 (4)	0.0023 (4)	0.0037 (4)
C6	0.0140 (5)	0.0120 (5)	0.0125 (5)	−0.0014 (4)	0.0017 (4)	0.0008 (4)
C7	0.0132 (5)	0.0137 (5)	0.0123 (5)	0.0001 (4)	0.0010 (4)	0.0005 (4)
C8	0.0165 (6)	0.0124 (5)	0.0162 (6)	0.0009 (4)	0.0012 (4)	0.0001 (4)
C9	0.0179 (6)	0.0160 (6)	0.0151 (6)	−0.0037 (5)	0.0017 (4)	−0.0021 (4)

C10	0.0151 (5)	0.0201 (6)	0.0156 (6)	−0.0011 (5)	−0.0009 (4)	−0.0014 (5)
C11	0.0147 (5)	0.0156 (6)	0.0168 (6)	0.0018 (4)	−0.0003 (4)	0.0003 (4)
C12	0.0134 (5)	0.0134 (5)	0.0134 (5)	0.0001 (4)	0.0012 (4)	−0.0004 (4)
C13	0.0132 (5)	0.0122 (5)	0.0138 (5)	0.0000 (4)	−0.0010 (4)	−0.0006 (4)
C14	0.0147 (5)	0.0157 (6)	0.0160 (6)	0.0008 (4)	0.0006 (4)	−0.0001 (5)
C15	0.0186 (6)	0.0199 (6)	0.0142 (5)	−0.0025 (5)	0.0022 (5)	0.0006 (5)
C16	0.0248 (6)	0.0138 (6)	0.0163 (6)	−0.0021 (5)	0.0003 (5)	0.0013 (5)
C17	0.0233 (6)	0.0122 (6)	0.0196 (6)	0.0040 (5)	0.0017 (5)	0.0005 (5)
C18	0.0159 (5)	0.0132 (5)	0.0147 (5)	0.0000 (4)	0.0015 (4)	−0.0005 (4)
C19	0.0147 (5)	0.0130 (6)	0.0156 (6)	−0.0010 (4)	0.0010 (4)	−0.0002 (4)
C20	0.0167 (6)	0.0154 (6)	0.0202 (6)	0.0030 (5)	0.0025 (5)	−0.0024 (5)
C21	0.0156 (6)	0.0223 (6)	0.0170 (6)	−0.0022 (5)	0.0035 (4)	−0.0048 (5)
C22	0.0188 (6)	0.0208 (6)	0.0152 (6)	−0.0029 (5)	0.0017 (5)	0.0015 (5)
C23	0.0151 (5)	0.0154 (6)	0.0173 (6)	−0.0005 (4)	−0.0015 (4)	0.0010 (5)
C24	0.0129 (5)	0.0126 (5)	0.0141 (5)	−0.0005 (4)	−0.0007 (4)	−0.0018 (4)

Geometric parameters (Å, °)

Si1—C12	1.847 (1)	C10—C11	1.382 (2)
Si1—C13	1.850 (1)	C10—H10	0.9500
Si1—C1	1.852 (1)	C11—C12	1.408 (2)
Si1—C24	1.857 (1)	C11—H11	0.9500
O1—C6	1.382 (1)	C13—C18	1.394 (2)
O1—C7	1.382 (1)	C13—C14	1.412 (2)
O2—C19	1.383 (2)	C14—C15	1.385 (2)
O2—C18	1.385 (2)	C14—H14	0.9500
C1—C6	1.399 (2)	C15—C16	1.395 (2)
C1—C2	1.410 (2)	C15—H15	0.9500
C2—C3	1.384 (2)	C16—C17	1.381 (2)
C2—H2	0.9500	C16—H16	0.9500
C3—C4	1.396 (2)	C17—C18	1.399 (2)
C3—H3	0.9500	C17—H17	0.9500
C4—C5	1.382 (2)	C19—C24	1.397 (2)
C4—H4	0.9500	C19—C20	1.399 (2)
C5—C6	1.401 (2)	C20—C21	1.383 (2)
C5—H5	0.9500	C20—H20	0.9500
C7—C8	1.397 (2)	C21—C22	1.394 (2)
C7—C12	1.401 (2)	C21—H21	0.9500
C8—C9	1.386 (2)	C22—C23	1.386 (2)
C8—H8	0.9500	C22—H22	0.9500
C9—C10	1.392 (2)	C23—C24	1.407 (2)
C9—H9	0.9500	C23—H23	0.9500
C12—Si1—C13	115.69 (6)	C12—C11—H11	118.8
C12—Si1—C1	100.57 (6)	C7—C12—C11	116.8 (1)
C13—Si1—C1	114.41 (5)	C7—C12—Si1	121.41 (9)
C12—Si1—C24	111.85 (5)	C11—C12—Si1	121.70 (9)
C13—Si1—C24	100.31 (6)	C18—C13—C14	116.6 (1)
C1—Si1—C24	114.70 (5)	C18—C13—Si1	121.32 (9)
C6—O1—C7	125.07 (9)	C14—C13—Si1	122.01 (9)

C19—O2—C18	124.5 (1)	C15—C14—C13	122.2 (1)
C6—C1—C2	116.8 (1)	C15—C14—H14	118.9
C6—C1—Si1	121.34 (9)	C13—C14—H14	118.9
C2—C1—Si1	121.90 (9)	C14—C15—C16	119.3 (1)
C3—C2—C1	122.2 (1)	C14—C15—H15	120.3
C3—C2—H2	118.9	C16—C15—H15	120.3
C1—C2—H2	118.9	C17—C16—C15	120.3 (1)
C2—C3—C4	119.4 (1)	C17—C16—H16	119.8
C2—C3—H3	120.3	C15—C16—H16	119.8
C4—C3—H3	120.3	C16—C17—C18	119.6 (1)
C5—C4—C3	120.3 (1)	C16—C17—H17	120.2
C5—C4—H4	119.9	C18—C17—H17	120.2
C3—C4—H4	119.9	O2—C18—C13	125.7 (1)
C4—C5—C6	119.66 (11)	O2—C18—C17	112.3 (1)
C4—C5—H5	120.2	C13—C18—C17	122.0 (1)
C6—C5—H5	120.2	O2—C19—C24	125.3 (1)
O1—C6—C1	125.5 (1)	O2—C19—C20	112.7 (1)
O1—C6—C5	112.7 (1)	C24—C19—C20	122.0 (1)
C1—C6—C5	121.7 (1)	C21—C20—C19	119.7 (1)
O1—C7—C8	113.1 (1)	C21—C20—H20	120.2
O1—C7—C12	125.3 (1)	C19—C20—H20	120.2
C8—C7—C12	121.6 (1)	C20—C21—C22	120.3 (1)
C9—C8—C7	119.6 (1)	C20—C21—H21	119.9
C9—C8—H8	120.2	C22—C21—H21	119.9
C7—C8—H8	120.2	C23—C22—C21	119.1 (1)
C8—C9—C10	120.4 (1)	C23—C22—H22	120.5
C8—C9—H9	119.8	C21—C22—H22	120.5
C10—C9—H9	119.8	C22—C23—C24	122.7 (1)
C11—C10—C9	119.2 (1)	C22—C23—H23	118.7
C11—C10—H10	120.4	C24—C23—H23	118.7
C9—C10—H10	120.4	C19—C24—C23	116.4 (1)
C10—C11—C12	122.4 (1)	C19—C24—Si1	121.43 (9)
C10—C11—H11	118.8	C23—C24—Si1	122.12 (9)

Interplanar angles (°)

Plane[a]	Plane	Dihedral angle
1	2	86.14 (3)
3	4	5.66 (4)
5	6	9.30 (5)
7	8	6.54 (6)

Note: (*a*) atoms defining planes: (1) Si1/O1/C1/C6/C7/C12; (2) Si1/O2/C13/C18/C19/C24; (3) Si1/O1/C1–C6; (4) Si1/O1/C7–C12; (5) Si1/O2/C13–C18; (6) Si1/O2/C19–C24; (7) C1–C6; (8) C7–C12 at (2 − *x*, 1 − *y*, −*z*).

Intermolecular contacts (Å)

Contact	Distance
Cg(7)···*Cg*(8)[a,b]	3.96
d(8···9)[c]	3.34

C15—H15···*Cg*(9)		2.68

Notes: (*a*) atoms defining planes: (7) C1–C6; (8) C7–C12 at (2 − *x*, 1 − *y*, −*z*); (9) C1–C6 at (*x*, 1.5 + *y*, −1/2 + *z*); (*b*) *Cg* = center of gravity of specified ring; (*c*) perpendicular distance between specified rings.

Fig. 1

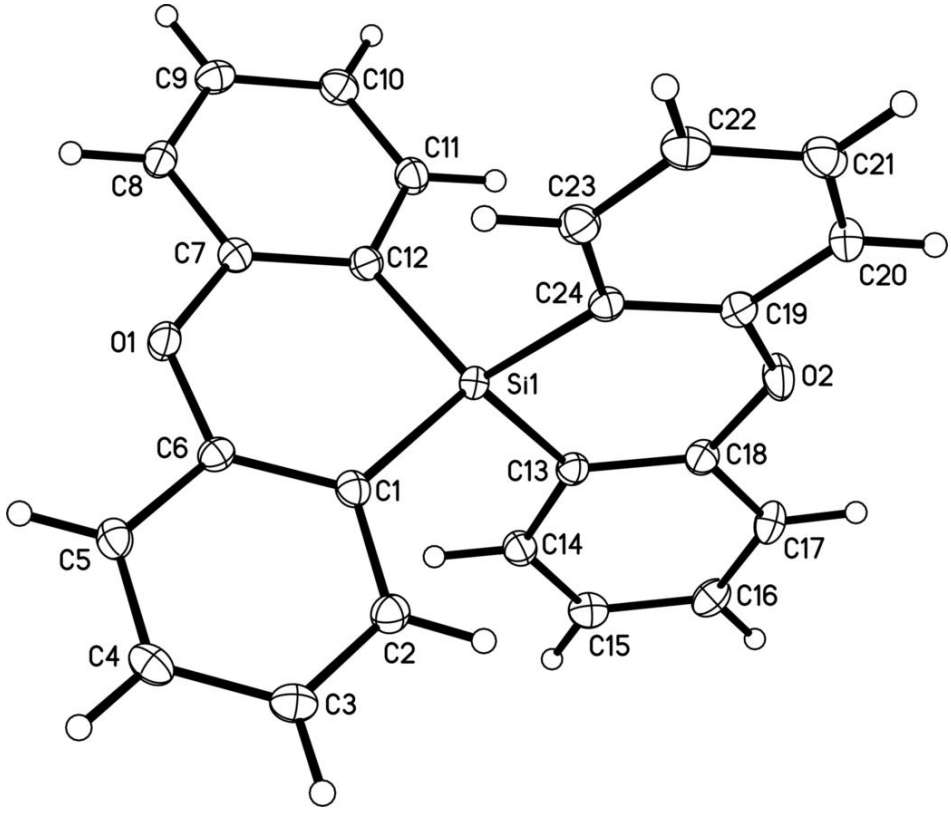
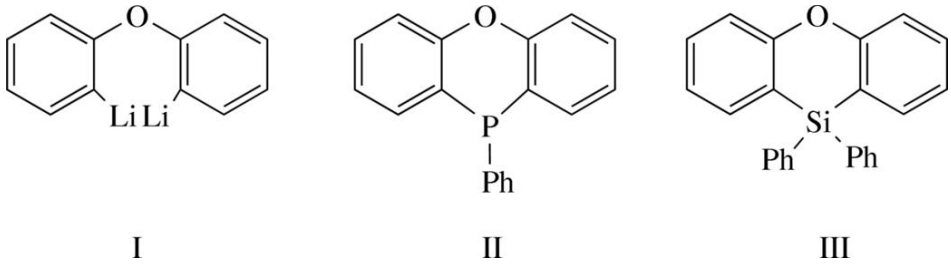

C9
C10
C11
C8
C7
C12
O1
C6
C1
C5
C4
C2
C3
Si1
C22
C21
C23
C20
C24
C19
O2
C18
C13
C14
C17
C16
C15

Fig. 2



I II III