

(*E,E*)-4,4'-Bis[dimethyl(styryl)silyl]-biphenyl

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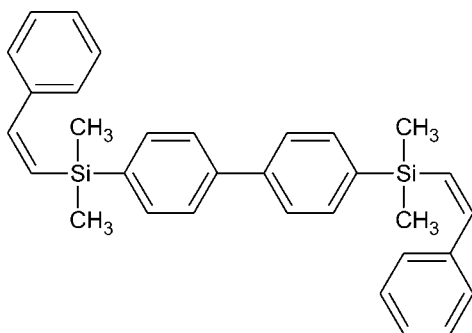
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; disorder in main residue; R factor = 0.040; wR factor = 0.065; data-to-parameter ratio = 14.1.

The molecule of the title compound, $\text{C}_{32}\text{H}_{34}\text{Si}_2$, occupies a special position of inversion symmetry. The biphenyl unit is disordered over two positions [with occupancies of 0.602 (11) and 0.398 (11)], the two phenylene rings being rotated by ca 25°. The dihedral angles between the phenylene and terminal phenyl rings are 50.9 (2) and 39.8 (3)° for the two alternative orientations of the biphenyl unit.

Related literature

For the synthesis of [(*E,E*)-2-bis(silyl)ethenyl]arenes, see: Itami *et al.* (2003); Majchrzak *et al.* (2005, 2007); Marciniak (2005, 2007); Marciniak & Pietraszuk (2003).



Experimental

Crystal data

$\text{C}_{32}\text{H}_{34}\text{Si}_2$	$V = 1324.4$ (3) Å ³
$M_r = 474.77$	$Z = 2$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 14.2037$ (16) Å	$\mu = 0.15$ mm ⁻¹
$b = 5.8647$ (8) Å	$T = 100$ (1) K
$c = 15.9022$ (16) Å	$0.2 \times 0.15 \times 0.1$ mm
$\beta = 91.111$ (9)°	

Data collection

Kuma KM-4 CCD diffractometer	3423 independent reflections
Absorption correction: none	1870 reflections with $I > 2\sigma(I)$
8939 measured reflections	$R_{\text{int}} = 0.050$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.065$	
$S = 0.88$	$\Delta\rho_{\text{max}} = 0.23$ e Å ⁻³
3423 reflections	$\Delta\rho_{\text{min}} = -0.25$ e Å ⁻³
243 parameters	

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1989); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2387).

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supplementary materials

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(*E,E*)-4,4'-Bis[dimethyl(styryl)silyl]biphenyl

M. Majchrzak, B. Marciniak and M. Kubicki

Comment

The title compound **1** (Scheme 1) was obtained by the highly efficient, stereo-selective silylative cross-coupling reaction catalysed by five coordination ruthenium hydride catalyst. This type of coupling reaction was discovered in the presence of transition metal complexes (*e.g.* ruthenium or rhodium) in which the metal-hydrogen [M—H] and metal-silicon [M—Si] bonds were initially introduced or generated in the solution (Marciniak, 2005, 2007; Marciniak & Pietraszuk, 2003). The above mentioned process has become an excellent method for the selective synthesis of new class of {(*E,E*)-2-bis(silyl)ethenyl}arenes (Majchrzak, *et al.* 2005, 2007; Itami, *et al.* 2003), and of molecular and macromolecular organosilicon compounds containing aromatic fragments which can be used as a potential photo- or optoelectronic material.

The molecules of 4,4'-bis{((*E*)-2-phenylethenyl)dimethylsilyl}biphenyl occupy the special positions, on the centers of symmetry in the space group P21/n. As a consequence, the symmetry-related aromatic rings are coplanar, in particular the central biphenyl fragment is coplanar. This fragment is disordered over two orientations (Fig. 2), their s.o.f.'s refined at 0.61 (1) and 0.39 (1). The successful anisotropic refinement of both alternative positions can be regarded as the proof of the appropriateness of the model used. The dihedral angle between the mean planes of the disordered rings is 24.8 (5)°. The overall conformation of the molecule may be described by the dihedral angles between three planar fragments (central and terminal phenyl rings, and the Si—C=C bridge). It turns out that the terminal ring is almost coplanar with the bridge (5.1 (2)°), while the central ring is significantly twisted, by 50.9 (2)° [39.8 (3) for less occupied position], with respect to the plane of the terminal ring.

The crystal structure is determined by van der Waals forces (Fig. 3), weak C—H... π contacts are the only possible specific interactions.

Experimental

[(*E,E*)-4,4'-bis(dimethyl(styryl)silyl)]biphenyl was synthesized according to the following procedure: 3.1 mg (0.00427 mmol) of ruthenium (II) - [RuHCl(CO)(PCy₃)₂], dried toluene (0.75M solution), 0.275 g (0.85 mmol) of 4,4'-bis(vinyldimethylsilyl)biphenyl and 0.181 g (1.74 mmol) of styrene were placed in 5 ml glass-mini reactor with reflux condenser connected with argon line. The reaction mixture was stirred and heated at 80°C (353 K) under an argon flow for 18 h. After the reaction was completed, the mixture was cooled to room temperature. Then the excess of organic solvent and styrene were evaporated and the residue was separated by column chromatography with silica gel (eluent - benzene/hexane) to afford pure product as white crystals which were washed by cool, dry ethanol twice (2 x 5 ml), filtrated and dried under high vacuum (0.379 g, yield 94%). ¹H NMR (CDCl₃, δ (p.p.m.)): 0.48 (s, 12H, —CH₃), 6.62 (d, 1H, J_{HH} = 18.9 Hz, Si—CH=CH—C₆H₅), 6.99 (d, 1H, J_{HH} = 19.8 Hz, Si—CH=CH—C₆H₅), 7.28–7.38 (m, 10H, *m,p*-C₆H₅), 7.49 (d, 4H, J_{HH} = 7.5 Hz, *o*-C₆H₅), 7.63–7.65 (q, 8H, —C₆H₄—C₆H₄). ¹³C NMR (CDCl₃; δ (p.p.m.)): -2.3 (—CH₃), 12 (*m*-C₆H₄), 126.5 (*p*-C₆H₅), 126.9 SiCH=CH—C<), 128.1 (*o*-C₆H₅), 128.4 (*m*-C₆H₅), 134.3 (*o*-C₆H₄), 137.4 (>C_i—C_i<), 138.0 (SiCH=CH—C<), 141.6 (>C—SiCH=CH—), 145.3 (Si—CH=CH—C<). ²⁹Si NMR (CDCl₃, δ (p.p.m.)): -10.05. HRMS (*M*/

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z) Calcd for $C_{32}H_{34}Si_2$: 474.21990, found: 474.21976. Anal. Calcd for $C_{32}H_{34}Si_2$: C 80.95, H 7.22, found: C 80.35, H 7.24. m. p. 131–132.0°C (404–405 K).

Refinement

Hydrogen atoms were found in difference Fourier maps and freely refined; only those from disordered part were located geometrically and refined as the 'riding model', with U_{iso} 's set at 1.2 times U_{eq} 's of their appropriate carrier atoms.

Figures

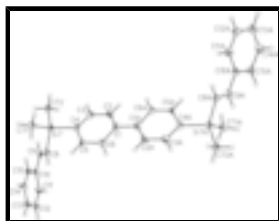


Fig. 1. Anisotropic displacement ellipsoid representation of the molecule **1** (at the 50% probability level), together with numbering scheme. The hydrogen atoms are drawn as spheres with arbitrary radii. For clarity, only the higher occupancy position is shown. Index A denotes the symmetry code $-x, 1 - y, 2 - z$.

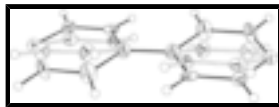


Fig. 2. Two alternative conformations of the central biphenyl fragment. The less-occupied fragment is drawn with open lines.

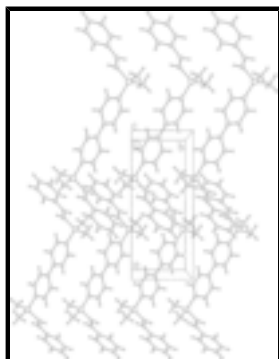


Fig. 3. The crystal packing as seen along c -direction.

(*E,E*)-4,4'-Bis[dimethyl(styryl)silyl]biphenyl

Crystal data

$C_{32}H_{34}Si_2$

$M_r = 474.77$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1n$

$a = 14.2037\ (16)\ \text{\AA}$

$b = 5.8647\ (8)\ \text{\AA}$

$c = 15.9022\ (16)\ \text{\AA}$

$\beta = 91.111\ (9)^\circ$

$V = 1324.4\ (3)\ \text{\AA}^3$

$Z = 2$

$F_{000} = 508$

$D_x = 1.191\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2358 reflections

$\theta = 2.6\text{--}29.4^\circ$

$\mu = 0.15\ \text{mm}^{-1}$

$T = 100\ (1)\ \text{K}$

Prism, colourless

$0.2 \times 0.15 \times 0.1\ \text{mm}$

Data collection

Kuma KM-4 CCD four-circle diffractometer	1870 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\text{int}} = 0.050$
Monochromator: graphite	$\theta_{\text{max}} = 29.5^\circ$
$T = 100(1)$ K	$\theta_{\text{min}} = 3.7^\circ$
ω scan	$h = -18 \rightarrow 13$
Absorption correction: none	$k = -8 \rightarrow 7$
8939 measured reflections	$l = -21 \rightarrow 20$
3423 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.040$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.065$	$w = 1/[\sigma^2(F_o^2) + (0.022P)^2]$
$S = 0.88$	where $P = (F_o^2 + 2F_c^2)/3$
3423 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
243 parameters	$\Delta\rho_{\text{max}} = 0.23 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.25 \text{ e } \text{\AA}^{-3}$
	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 $F^2 > 2\sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.04302 (10)	0.4397 (3)	0.98598 (9)	0.0230 (4)	
C2A	0.0429 (3)	0.2834 (10)	0.9213 (4)	0.0261 (12)	0.602 (11)
H2A	-0.0145	0.2548	0.8915	0.031*	0.602 (11)
C3A	0.1232 (3)	0.1656 (10)	0.8981 (4)	0.0250 (11)	0.602 (11)
H3A	0.1183	0.0565	0.8541	0.030*	0.602 (11)

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C5A	0.2145 (8)	0.375 (2)	0.9944 (7)	0.0186 (15)	0.602 (11)
H5A	0.2745	0.4116	1.0181	0.022*	0.602 (11)
C6A	0.1349 (10)	0.499 (2)	1.0201 (6)	0.0176 (15)	0.602 (11)
H6A	0.1416	0.6208	1.0593	0.021*	0.602 (11)
C2B	0.0323 (4)	0.2057 (13)	0.9541 (5)	0.0197 (15)	0.398 (11)
H2B	-0.0276	0.1337	0.9519	0.024*	0.398 (11)
C3B	0.1116 (5)	0.0938 (14)	0.9276 (5)	0.0204 (15)	0.398 (11)
H3B	0.1055	-0.0542	0.9038	0.024*	0.398 (11)
C5B	0.2057 (13)	0.412 (3)	0.9760 (10)	0.018 (2)	0.398 (11)
H5B	0.2642	0.4834	0.9887	0.021*	0.398 (11)
C6B	0.1267 (14)	0.520 (3)	0.9981 (8)	0.015 (2)	0.398 (11)
H6B	0.1329	0.6649	1.0244	0.018*	0.398 (11)
C4	0.20746 (10)	0.2006 (2)	0.93548 (9)	0.0197 (4)	
Si7	0.31611 (3)	0.03985 (7)	0.90780 (3)	0.02026 (13)	
C71	0.36430 (13)	-0.0933 (3)	1.00630 (11)	0.0259 (4)	
H71A	0.4143 (11)	-0.192 (3)	0.9951 (9)	0.035 (5)*	
H71B	0.3889 (11)	0.021 (3)	1.0449 (10)	0.048 (5)*	
H71C	0.3169 (11)	-0.179 (2)	1.0367 (9)	0.034 (5)*	
C72	0.28878 (13)	-0.1761 (3)	0.82585 (11)	0.0237 (4)	
H72A	0.2639 (11)	-0.108 (3)	0.7761 (11)	0.051 (6)*	
H72B	0.2440 (10)	-0.285 (3)	0.8472 (9)	0.034 (5)*	
H72C	0.3448 (11)	-0.260 (3)	0.8101 (9)	0.036 (5)*	
C8	0.40637 (11)	0.2437 (3)	0.87160 (11)	0.0217 (4)	
H8	0.4218 (9)	0.367 (2)	0.9091 (9)	0.029 (4)*	
C9	0.45509 (11)	0.2270 (3)	0.80126 (10)	0.0210 (4)	
H9	0.4419 (9)	0.103 (2)	0.7636 (8)	0.020 (4)*	
C10	0.53036 (10)	0.3781 (3)	0.77198 (9)	0.0202 (4)	
C11	0.55571 (11)	0.5802 (3)	0.81306 (11)	0.0269 (4)	
H11	0.5212 (10)	0.623 (3)	0.8614 (10)	0.037 (5)*	
C12	0.62683 (12)	0.7157 (3)	0.78294 (11)	0.0283 (4)	
H12	0.6422 (9)	0.853 (2)	0.8108 (9)	0.024 (4)*	
C13	0.67546 (11)	0.6525 (3)	0.71236 (10)	0.0259 (4)	
H13	0.7258 (10)	0.751 (2)	0.6914 (8)	0.026 (4)*	
C14	0.65094 (11)	0.4553 (3)	0.67053 (10)	0.0243 (4)	
H14	0.6841 (9)	0.405 (2)	0.6204 (9)	0.024 (4)*	
C15	0.57906 (11)	0.3194 (3)	0.70024 (10)	0.0222 (4)	
H15	0.5628 (10)	0.182 (2)	0.6712 (9)	0.029 (5)*	

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0210 (9)	0.0264 (9)	0.0214 (9)	0.0060 (8)	-0.0036 (7)	-0.0053 (8)
C2A	0.0147 (18)	0.033 (3)	0.030 (3)	-0.0006 (17)	-0.0054 (17)	-0.011 (2)
C3A	0.024 (2)	0.028 (3)	0.024 (3)	0.0003 (18)	0.0041 (19)	-0.014 (2)
C5A	0.012 (2)	0.020 (4)	0.023 (4)	0.006 (2)	0.000 (2)	0.005 (2)
C6A	0.020 (2)	0.024 (3)	0.008 (3)	0.0013 (19)	-0.004 (3)	0.001 (2)
C2B	0.011 (2)	0.024 (3)	0.025 (4)	-0.001 (2)	0.000 (2)	0.002 (3)
C3B	0.019 (3)	0.018 (3)	0.024 (4)	-0.003 (2)	-0.001 (3)	-0.003 (3)

C5B	0.016 (4)	0.006 (4)	0.030 (6)	-0.004 (3)	-0.004 (4)	0.006 (4)
C6B	0.025 (5)	0.010 (3)	0.012 (6)	0.000 (3)	0.004 (4)	-0.002 (4)
C4	0.0208 (9)	0.0229 (9)	0.0153 (8)	0.0044 (7)	-0.0009 (7)	-0.0003 (7)
Si7	0.0186 (2)	0.0217 (2)	0.0205 (2)	0.0040 (2)	-0.00016 (17)	-0.0026 (2)
C71	0.0232 (10)	0.0292 (11)	0.0251 (10)	0.0039 (9)	-0.0011 (8)	-0.0026 (8)
C72	0.0228 (10)	0.0255 (10)	0.0227 (10)	0.0056 (8)	0.0008 (8)	-0.0033 (8)
C8	0.0202 (9)	0.0204 (9)	0.0243 (10)	0.0039 (7)	-0.0026 (7)	-0.0028 (8)
C9	0.0216 (9)	0.0188 (9)	0.0226 (9)	0.0037 (7)	-0.0028 (7)	-0.0028 (8)
C10	0.0184 (8)	0.0221 (9)	0.0201 (9)	0.0057 (7)	-0.0030 (7)	0.0003 (7)
C11	0.0263 (10)	0.0285 (10)	0.0259 (10)	0.0018 (8)	0.0039 (8)	-0.0069 (8)
C12	0.0285 (10)	0.0251 (10)	0.0313 (11)	-0.0034 (8)	-0.0026 (8)	-0.0061 (8)
C13	0.0222 (9)	0.0289 (10)	0.0264 (10)	-0.0023 (8)	-0.0046 (8)	0.0047 (8)
C14	0.0222 (9)	0.0295 (9)	0.0211 (9)	0.0040 (8)	-0.0005 (7)	0.0014 (8)
C15	0.0220 (9)	0.0219 (9)	0.0225 (9)	0.0020 (8)	-0.0024 (7)	-0.0017 (8)

Geometric parameters (Å, °)

C1—C6B	1.29 (2)	Si7—C72	1.8530 (17)
C1—C2A	1.377 (4)	Si7—C71	1.8682 (17)
C1—C6A	1.446 (12)	C71—H71A	0.935 (15)
C1—C2B	1.470 (7)	C71—H71B	0.969 (17)
C1—C1 ⁱ	1.488 (3)	C71—H71C	0.976 (16)
C2A—C3A	1.390 (6)	C72—H72A	0.948 (17)
C2A—H2A	0.9500	C72—H72B	0.969 (15)
C3A—C4	1.342 (5)	C72—H72C	0.971 (15)
C3A—H3A	0.9500	C8—C9	1.330 (2)
C5A—C4	1.390 (13)	C8—H8	0.962 (14)
C5A—C6A	1.412 (19)	C9—C10	1.471 (2)
C5A—H5A	0.9500	C9—H9	0.957 (13)
C6A—H6A	0.9500	C10—C15	1.389 (2)
C2B—C3B	1.377 (9)	C10—C11	1.397 (2)
C2B—H2B	0.9500	C11—C12	1.378 (2)
C3B—C4	1.502 (8)	C11—H11	0.954 (15)
C3B—H3B	0.9500	C12—C13	1.380 (2)
C5B—C6B	1.34 (3)	C12—H12	0.942 (14)
C5B—C4	1.396 (19)	C13—C14	1.376 (2)
C5B—H5B	0.9500	C13—H13	0.982 (14)
C6B—H6B	0.9500	C14—C15	1.385 (2)
C4—Si7	1.8682 (15)	C14—H14	0.978 (14)
Si7—C8	1.8528 (17)	C15—H15	0.953 (14)
C2A—C1—C6A	115.4 (5)	C8—Si7—C4	109.11 (7)
C6B—C1—C2B	118.8 (8)	C72—Si7—C4	110.36 (8)
C6B—C1—C1 ⁱ	122.8 (8)	C71—Si7—C4	107.72 (8)
C2A—C1—C1 ⁱ	123.4 (2)	Si7—C71—H71A	111.5 (9)
C6A—C1—C1 ⁱ	120.8 (5)	Si7—C71—H71B	111.3 (9)
C2B—C1—C1 ⁱ	117.8 (3)	H71A—C71—H71B	106.4 (13)
C1—C2A—C3A	122.7 (4)	Si7—C71—H71C	112.7 (9)
C1—C2A—H2A	118.7	H71A—C71—H71C	108.1 (13)

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C3A—C2A—H2A	118.7	H71B—C71—H71C	106.6 (13)
C4—C3A—C2A	122.4 (4)	Si7—C72—H72A	111.6 (10)
C4—C3A—H3A	118.8	Si7—C72—H72B	109.6 (9)
C2A—C3A—H3A	118.8	H72A—C72—H72B	109.5 (13)
C4—C5A—C6A	121.8 (10)	Si7—C72—H72C	111.4 (9)
C4—C5A—H5A	119.1	H72A—C72—H72C	106.9 (13)
C6A—C5A—H5A	119.1	H72B—C72—H72C	107.6 (13)
C5A—C6A—C1	119.2 (10)	C9—C8—Si7	126.02 (13)
C5A—C6A—H6A	120.4	C9—C8—H8	117.4 (9)
C1—C6A—H6A	120.4	Si7—C8—H8	116.5 (9)
C3B—C2B—C1	118.1 (5)	C8—C9—C10	127.94 (16)
C3B—C2B—H2B	121.0	C8—C9—H9	118.9 (8)
C1—C2B—H2B	121.0	C10—C9—H9	113.2 (8)
C2B—C3B—C4	121.4 (5)	C15—C10—C11	117.79 (15)
C2B—C3B—H3B	119.3	C15—C10—C9	119.17 (15)
C4—C3B—H3B	119.3	C11—C10—C9	123.04 (15)
C6B—C5B—C4	124.3 (15)	C12—C11—C10	120.70 (16)
C6B—C5B—H5B	117.8	C12—C11—H11	121.3 (9)
C4—C5B—H5B	117.8	C10—C11—H11	118.0 (9)
C1—C6B—C5B	124.1 (15)	C11—C12—C13	120.63 (17)
C1—C6B—H6B	118.0	C11—C12—H12	119.6 (9)
C5B—C6B—H6B	118.0	C13—C12—H12	119.8 (9)
C3A—C4—C5A	117.6 (5)	C14—C13—C12	119.54 (17)
C5B—C4—C3B	112.6 (8)	C14—C13—H13	120.6 (8)
C3A—C4—Si7	123.5 (2)	C12—C13—H13	119.8 (8)
C5A—C4—Si7	118.8 (5)	C13—C14—C15	120.01 (17)
C5B—C4—Si7	125.3 (7)	C13—C14—H14	121.6 (8)
C3B—C4—Si7	121.4 (3)	C15—C14—H14	118.3 (8)
C8—Si7—C72	111.06 (8)	C14—C15—C10	121.31 (16)
C8—Si7—C71	106.60 (8)	C14—C15—H15	119.6 (9)
C72—Si7—C71	111.85 (9)	C10—C15—H15	119.1 (9)
C6B—C1—C2A—C3A	23.9 (7)	C6B—C5B—C4—Si7	-177.3 (9)
C6A—C1—C2A—C3A	8.9 (6)	C2B—C3B—C4—C3A	-82.3 (10)
C2B—C1—C2A—C3A	-89.8 (8)	C2B—C3B—C4—C5A	20.6 (6)
C1 ⁱ —C1—C2A—C3A	-177.5 (3)	C2B—C3B—C4—C5B	3.5 (7)
C1—C2A—C3A—C4	-1.9 (5)	C2B—C3B—C4—Si7	174.9 (4)
C4—C5A—C6A—C1	1.8 (12)	C3A—C4—Si7—C8	120.2 (4)
C6B—C1—C6A—C5A	-80 (5)	C5A—C4—Si7—C8	-55.9 (4)
C2A—C1—C6A—C5A	-8.7 (9)	C5B—C4—Si7—C8	-38.9 (7)
C2B—C1—C6A—C5A	23.3 (9)	C3B—C4—Si7—C8	150.9 (4)
C1 ⁱ —C1—C6A—C5A	177.5 (6)	C3A—C4—Si7—C72	-2.1 (4)
C6B—C1—C2B—C3B	-8.9 (8)	C5A—C4—Si7—C72	-178.2 (4)
C2A—C1—C2B—C3B	70.2 (8)	C5B—C4—Si7—C72	-161.2 (7)
C6A—C1—C2B—C3B	-25.4 (7)	C3B—C4—Si7—C72	28.6 (4)
C1 ⁱ —C1—C2B—C3B	179.6 (4)	C3A—C4—Si7—C71	-124.4 (4)
C1—C2B—C3B—C4	3.6 (7)	C5A—C4—Si7—C71	59.4 (4)
C2A—C1—C6B—C5B	-23.4 (13)	C5B—C4—Si7—C71	76.4 (7)
C6A—C1—C6B—C5B	91 (5)	C3B—C4—Si7—C71	-93.8 (4)

C2B—C1—C6B—C5B	6.7 (14)	C72—Si7—C8—C9	-7.84 (16)
C1 ⁱ —C1—C6B—C5B	177.8 (9)	C71—Si7—C8—C9	114.23 (14)
C4—C5B—C6B—C1	1.3 (19)	C4—Si7—C8—C9	-129.71 (13)
C2A—C3A—C4—C5A	-5.5 (6)	Si7—C8—C9—C10	-176.81 (12)
C2A—C3A—C4—C5B	-19.6 (7)	C8—C9—C10—C15	173.90 (15)
C2A—C3A—C4—C3B	84.4 (10)	C8—C9—C10—C11	-6.2 (2)
C2A—C3A—C4—Si7	178.3 (2)	C15—C10—C11—C12	0.0 (2)
C6A—C5A—C4—C3A	5.4 (10)	C9—C10—C11—C12	-179.98 (15)
C6A—C5A—C4—C5B	63 (4)	C10—C11—C12—C13	-1.1 (2)
C6A—C5A—C4—C3B	-23.2 (9)	C11—C12—C13—C14	1.7 (2)
C6A—C5A—C4—Si7	-178.2 (6)	C12—C13—C14—C15	-1.2 (2)
C6B—C5B—C4—C3A	20.9 (14)	C13—C14—C15—C10	0.1 (2)
C6B—C5B—C4—C5A	-107 (5)	C11—C10—C15—C14	0.5 (2)
C6B—C5B—C4—C3B	-6.3 (14)	C9—C10—C15—C14	-179.55 (14)

Symmetry codes: (i) $-x, -y+1, -z+2$.

Fig. 1

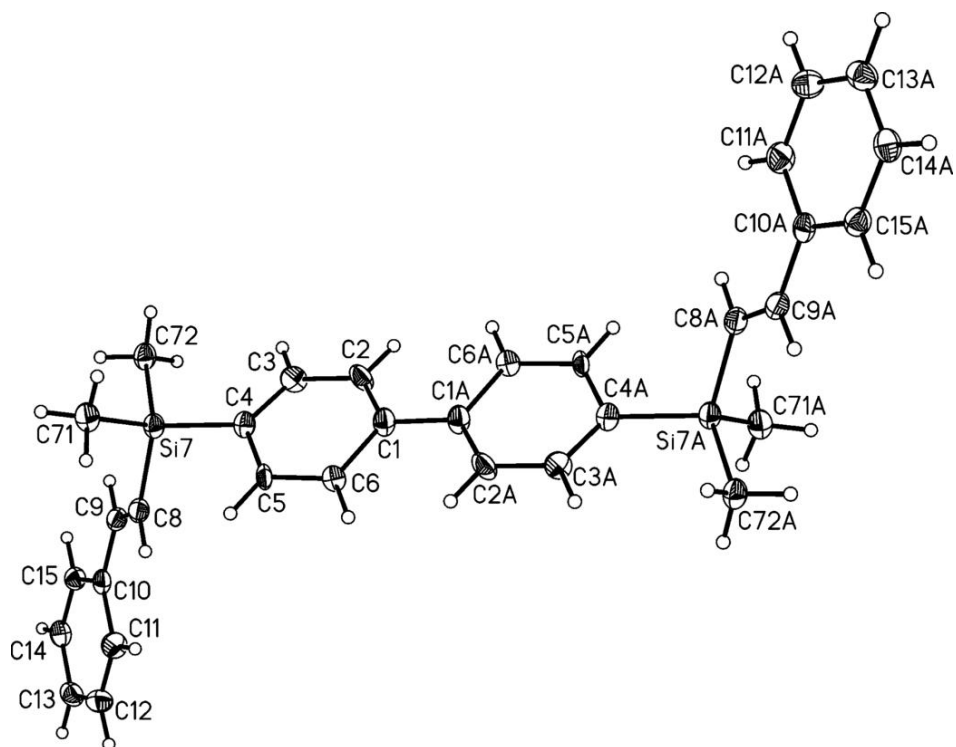


Fig. 2

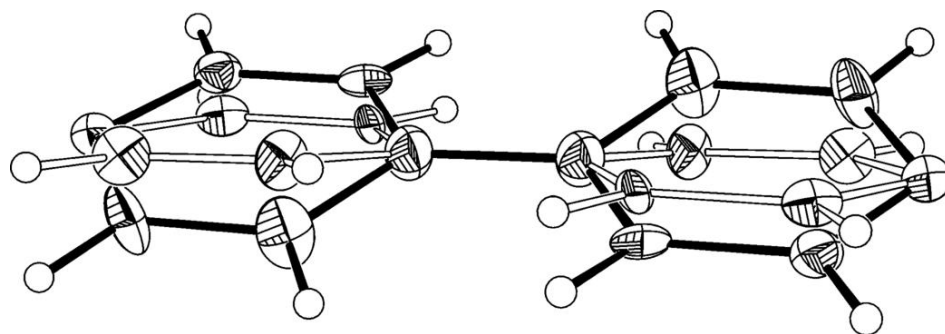


Fig. 3

