Acta Crystallographica Section E
**Structure Reports**
**Online**

ISSN 1600-5368

# 1,4-Bis[4-(dimethylsilyl)phenyl]benzene

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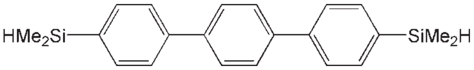
Received 24 February 2010; accepted 23 March 2010

Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.071; $wR$ factor = 0.133; data-to-parameter ratio = 19.3.

The complete molecule of the title compound, $C_{22}H_{26}Si_2$, is generated by a crystallographic centre of symmetry. The central benzene ring makes a dihedral angle of 26.7 (4)° with the 4-(dimethylsilyl)phenyl ring. There are weak C—H$\cdots\pi$ interactions in the crystal structure.

## Related literature

For applications of $p$-terphenyl derivatives as laser dyes, see: Craig *et al.* (1992), as light-emitting materials, see: Spiliopoulos *et al.* (2002) and as liquid crystalline materials, see: Yam *et al.* (1993). For a description of the Cambridge Structural Database, see: Allen (2002); Although $p$-terphenyls containing silyl groups have been reported (Feng *et al.*, 2007), their crystal structures have not yet been determined.



## Experimental

### *Crystal data*

$C_{22}H_{26}Si_2$
$M_r$ = 346.61
Monoclinic, $P2_1/c$
$a$ = 15.143 (3) Å
$b$ = 7.7263 (15) Å
$c$ = 9.1285 (18) Å
$\beta$ = 107.52 (3)°
$V$ = 1018.5 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.18 mm$^{-1}$
$T$ = 173 K
0.20 × 0.18 × 0.08 mm

### *Data collection*

Rigaku Saturn724+ CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)
$T_{min}$ = 0.966, $T_{max}$ = 0.986
7661 measured reflections
2218 independent reflections
1937 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.043

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.133
$S$ = 1.21
2218 reflections
115 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

$Cg$1 is the centroid of the C1–C6 ring.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C8—H8b$\cdots Cg1^{i}$ | 0.98 | 2.86 | 3.826 (3) | 171 |
| C10—H10a$\cdots Cg1^{ii}$ | 0.95 | 2.98 | 3.788 (3) | 143 |

Symmetry codes: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

This work was supported by the National Science Foundation of China (NSFC, Nos. 50673094 and 20774102).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FB2186).

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# supporting information

*Acta Cryst.* (2010). E**66**, o971 [doi:10.1107/S1600536810010883]

## 1,4-Bis[4-(dimethylsilyl)phenyl]benzene

**Lei Fang, Rui Wang, Li-Min Chen, Cai-Hong Xu and Shu-Hong Li**

### S1. Comment

*p*-Terphenyl derivatives have attracted considerable attention due to their extensive applications. Among others, they may be used as laser dyes (Craig *et al.*, 1992), light-emitting materials (Spiliopoulos *et al.*, 2002), liquid crystalline materials (Yam *et al.*, 1993). Although *p*-terphenyls containing silyl groups have been reported (Feng *et al.*, 2007), their crystal structures have not been given yet.

The title molecules are situated on the crystallographic centres of symmetry (Fig. 1). Two dimethylsilylphenyl-rings are linked to the central benzene ring in its 1,4 (*para*) positions. The rings are not coplanar; the dihedral angle between the dimethylsilylphenyl-ring and the central benzene ring equals to 26.7 (4)°. There are C-H···$\pi$-electron ring interactions in the structure (Tab. 1).

The distance Si1-H1 (1.39 (3)Å) is in a fair accordance to the structures with the R-factor < 0.06 that have been retrieved from the Cambridge Crystallographic Database (version 5.31 from December 2009 with updates up to February 2010). (Allen, 2002). The average retrieved distance is 1.419 (14) Å for 21 observations. [The searched structures contained Si-fragment as it is in the title structure: 2 C atoms in sp$^3$ state, 1 in sp$^2$ state, 1 H. The structures with extensively deviated distances (ROLDIF, ROLDIF01, POZNEX, CODVOH, YOYBOD) have been suppressed.]

### S2. Experimental

The reaction scheme is shown in Fig. 2. A solution of *n*-BuLi in hexane (1.6 M, 0.88 ml) was added dropwise to a solution of 1,4-bis(4-iodophenyl)benzene (192 mg, 0.40 mmol) in anhydrous tetrahydrofuran (THF) (80 ml) at -78 °C. After the solution having been stirred for 1 h, dimethylchlorosilane (152 mg, 1.60 mmol), also cooled to the same temperature, was added by syringe. The mixture was allowed to warm to room temperature and it was stirred overnight. After it had been quenched with saturated $NaHCO_3$ solution, the mixture was extracted with $Et_2O$. The organic layer was washed with brine, dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure. The mixture was recrystallized from ethanol to give 92 mg of the title product in 67% yield. The crystals were colourless needles with the average length of about 3 mm.

### S3. Refinement

All the hydrogens were discernible in the difference electron density maps. Nevertheless, all the hydrogens except the hydrogen attached to Si that was refined freely, were constrained by the riding-hydrogen formalism with $U_{iso}(H)=1.2U_{eq}(C_{aryl})$ or $U_{iso}(H)=1.5U_{eq}(C_{methyl})$. The C-H distances were constrained to 0.95 and 0.98 Å for the aryl and the methyl hydrogens, respectively.

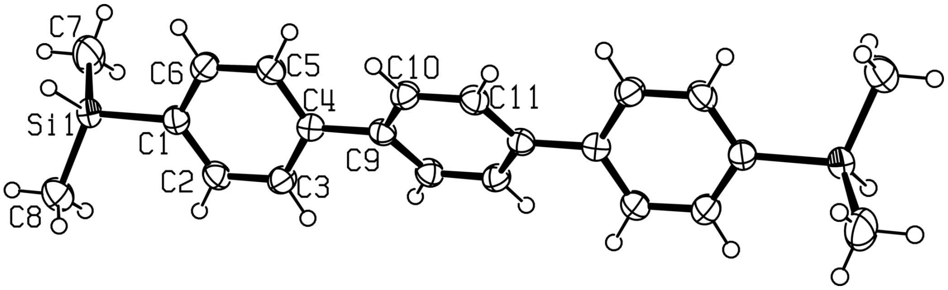

**Figure 1**

The title molecule, showing 50% probability displacement ellipsoids and the atom-numbering scheme. The atoms without labels are related to the labelled ones by -*x*, -*y*+1, -*z*+2.

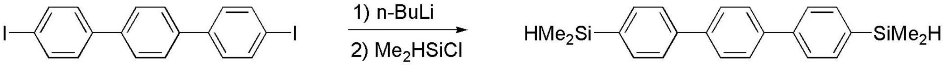

**Figure 2**

Reaction scheme for the synthesis of 1,4-bis(4-dimethylsilylphenyl)benzene

### 1,4-Bis[4-(dimethylsilyl)phenyl]benzene

*Crystal data*

$C_{22}H_{26}Si_2$
$M_r$ = 346.61
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 15.143 (3) Å
$b$ = 7.7263 (15) Å
$c$ = 9.1285 (18) Å
$\beta$ = 107.52 (3)°
$V$ = 1018.5 (3) Å$^3$
$Z$ = 2
$F(000)$ = 372
$D_x$ = 1.130 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 347 reflections
$\theta$ = 2.2–27.5°
$\mu$ = 0.18 mm$^{-1}$
$T$ = 173 K
Plate, colorless
0.20 × 0.18 × 0.08 mm

*Data collection*

Rigaku Saturn724+ CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans at fixed $\chi$ = 45°
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)
$T_{min}$ = 0.966, $T_{max}$ = 0.986
7661 measured reflections
2218 independent reflections
1937 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.043
$\theta_{max}$ = 27.0°, $\theta_{min}$ = 2.8°
$h = -19 \rightarrow 19$
$k = -9 \rightarrow 9$
$l = -7 \rightarrow 11$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.133
$S$ = 1.21
2218 reflections
115 parameters
0 restraints
46 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0276P)^2 + 0.8805P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.31$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.22$ e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{\rm iso}$*/$U_{\rm eq}$ |
|---|---|---|---|---|
| Si1 | 0.35065 (5) | 0.48948 (10) | 0.54899 (8) | 0.0361 (2) |
| C1 | 0.26293 (17) | 0.4896 (3) | 0.6572 (3) | 0.0312 (5) |
| C2 | 0.17225 (18) | 0.4309 (3) | 0.5939 (3) | 0.0341 (6) |
| H2A | 0.1533 | 0.3895 | 0.4911 | 0.041* |
| C3 | 0.10866 (17) | 0.4313 (3) | 0.6768 (3) | 0.0338 (6) |
| H3A | 0.0474 | 0.3906 | 0.6299 | 0.041* |
| C4 | 0.13394 (16) | 0.4907 (3) | 0.8282 (3) | 0.0288 (5) |
| C5 | 0.22485 (18) | 0.5474 (4) | 0.8935 (3) | 0.0357 (6) |
| H5A | 0.2441 | 0.5869 | 0.9968 | 0.043* |
| C6 | 0.28736 (18) | 0.5469 (4) | 0.8098 (3) | 0.0365 (6) |
| H6A | 0.3487 | 0.5866 | 0.8572 | 0.044* |
| C7 | 0.4368 (2) | 0.3127 (5) | 0.6203 (4) | 0.0660 (11) |
| H7A | 0.4832 | 0.3164 | 0.5651 | 0.099* |
| H7B | 0.4051 | 0.2006 | 0.6028 | 0.099* |
| H7C | 0.4674 | 0.3283 | 0.7305 | 0.099* |
| C8 | 0.2933 (2) | 0.4691 (4) | 0.3401 (3) | 0.0468 (7) |
| H8A | 0.2475 | 0.5617 | 0.3060 | 0.070* |
| H8B | 0.2624 | 0.3565 | 0.3182 | 0.070* |
| H8C | 0.3398 | 0.4785 | 0.2854 | 0.070* |
| C9 | 0.06529 (16) | 0.4952 (3) | 0.9166 (3) | 0.0292 (5) |
| C10 | 0.07421 (17) | 0.6139 (3) | 1.0364 (3) | 0.0319 (6) |
| H10A | 0.1249 | 0.6924 | 1.0622 | 0.038* |
| C11 | 0.01023 (17) | 0.6186 (3) | 1.1179 (3) | 0.0322 (6) |
| H11A | 0.0178 | 0.7004 | 1.1985 | 0.039* |
| H1 | 0.3948 (17) | 0.649 (3) | 0.578 (3) | 0.036 (7)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Si1 | 0.0341 (4) | 0.0455 (5) | 0.0312 (4) | −0.0040 (3) | 0.0137 (3) | 0.0030 (3) |
| C1 | 0.0319 (13) | 0.0320 (13) | 0.0314 (12) | 0.0010 (11) | 0.0119 (10) | 0.0015 (11) |
| C2 | 0.0384 (14) | 0.0381 (14) | 0.0266 (12) | −0.0009 (12) | 0.0113 (11) | −0.0023 (11) |
| C3 | 0.0295 (13) | 0.0366 (14) | 0.0345 (14) | −0.0019 (11) | 0.0085 (11) | −0.0027 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C4 | 0.0300 (12) | 0.0265 (12) | 0.0298 (12) | 0.0007 (10) | 0.0086 (9) | −0.0002 (10) |
| C5 | 0.0359 (14) | 0.0432 (16) | 0.0281 (13) | −0.0026 (12) | 0.0100 (10) | −0.0044 (11) |
| C6 | 0.0308 (13) | 0.0426 (15) | 0.0364 (14) | −0.0037 (12) | 0.0106 (11) | −0.0023 (12) |
| C7 | 0.0479 (19) | 0.094 (3) | 0.065 (2) | 0.0250 (19) | 0.0313 (17) | 0.026 (2) |
| C8 | 0.0528 (18) | 0.0535 (19) | 0.0370 (15) | −0.0004 (15) | 0.0178 (13) | −0.0022 (13) |
| C9 | 0.0294 (12) | 0.0298 (13) | 0.0280 (11) | 0.0030 (11) | 0.0079 (9) | 0.0045 (10) |
| C10 | 0.0295 (12) | 0.0337 (13) | 0.0319 (13) | −0.0033 (11) | 0.0082 (10) | −0.0032 (10) |
| C11 | 0.0351 (14) | 0.0331 (14) | 0.0287 (12) | −0.0025 (11) | 0.0101 (11) | −0.0037 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Si1—C8 | 1.848 (3) | C6—H6A | 0.9500 |
| Si1—C7 | 1.865 (3) | C7—H7A | 0.9800 |
| Si1—C1 | 1.879 (2) | C7—H7B | 0.9800 |
| Si1—H1 | 1.39 (3) | C7—H7C | 0.9800 |
| C1—C2 | 1.395 (3) | C8—H8A | 0.9800 |
| C1—C6 | 1.401 (3) | C8—H8B | 0.9800 |
| C2—C3 | 1.393 (3) | C8—H8C | 0.9800 |
| C2—H2A | 0.9500 | C9—C11$^{\text{i}}$ | 1.401 (3) |
| C3—C4 | 1.396 (3) | C9—C10 | 1.402 (3) |
| C3—H3A | 0.9500 | C10—C11 | 1.388 (3) |
| C4—C5 | 1.396 (3) | C10—H10A | 0.9500 |
| C4—C9 | 1.496 (3) | C11—C9$^{\text{i}}$ | 1.401 (3) |
| C5—C6 | 1.384 (3) | C11—H11A | 0.9500 |
| C5—H5A | 0.9500 | | |
| | | | |
| C8—Si1—C7 | 111.07 (16) | C1—C6—H6A | 119.0 |
| C8—Si1—C1 | 110.83 (12) | Si1—C7—H7A | 109.5 |
| C7—Si1—C1 | 110.34 (13) | Si1—C7—H7B | 109.5 |
| C8—Si1—H1 | 108.8 (10) | H7A—C7—H7B | 109.5 |
| C7—Si1—H1 | 109.7 (10) | Si1—C7—H7C | 109.5 |
| C1—Si1—H1 | 106.0 (10) | H7A—C7—H7C | 109.5 |
| C2—C1—C6 | 116.6 (2) | H7B—C7—H7C | 109.5 |
| C2—C1—Si1 | 123.04 (18) | Si1—C8—H8A | 109.5 |
| C6—C1—Si1 | 120.39 (19) | Si1—C8—H8B | 109.5 |
| C3—C2—C1 | 122.0 (2) | H8A—C8—H8B | 109.5 |
| C3—C2—H2A | 119.0 | Si1—C8—H8C | 109.5 |
| C1—C2—H2A | 119.0 | H8A—C8—H8C | 109.5 |
| C2—C3—C4 | 120.7 (2) | H8B—C8—H8C | 109.5 |
| C2—C3—H3A | 119.7 | C11$^{\text{i}}$—C9—C10 | 117.8 (2) |
| C4—C3—H3A | 119.7 | C11$^{\text{i}}$—C9—C4 | 121.1 (2) |
| C5—C4—C3 | 117.8 (2) | C10—C9—C4 | 121.1 (2) |
| C5—C4—C9 | 121.3 (2) | C11—C10—C9 | 121.1 (2) |
| C3—C4—C9 | 120.9 (2) | C11—C10—H10A | 119.5 |
| C6—C5—C4 | 121.0 (2) | C9—C10—H10A | 119.5 |
| C6—C5—H5A | 119.5 | C10—C11—C9$^{\text{i}}$ | 121.1 (2) |
| C4—C5—H5A | 119.5 | C10—C11—H11A | 119.4 |
| C5—C6—C1 | 122.0 (2) | C9$^{\text{i}}$—C11—H11A | 119.4 |

| | | | |
|---|---|---|---|
| C5—C6—H6A | 119.0 | | |

| | | | |
|---|---|---|---|
| C8—Si1—C1—C2 | 17.6 (3) | C4—C5—C6—C1 | −0.2 (4) |
| C7—Si1—C1—C2 | −105.9 (3) | C2—C1—C6—C5 | −0.7 (4) |
| C8—Si1—C1—C6 | −163.7 (2) | Si1—C1—C6—C5 | −179.4 (2) |
| C7—Si1—C1—C6 | 72.8 (3) | C5—C4—C9—C11$^{i}$ | −154.1 (2) |
| C6—C1—C2—C3 | 0.8 (4) | C3—C4—C9—C11$^{i}$ | 26.7 (4) |
| Si1—C1—C2—C3 | 179.6 (2) | C5—C4—C9—C10 | 26.2 (4) |
| C1—C2—C3—C4 | −0.2 (4) | C3—C4—C9—C10 | −153.1 (2) |
| C2—C3—C4—C5 | −0.7 (4) | C11$^{i}$—C9—C10—C11 | −0.1 (4) |
| C2—C3—C4—C9 | 178.6 (2) | C4—C9—C10—C11 | 179.7 (2) |
| C3—C4—C5—C6 | 0.9 (4) | C9—C10—C11—C9$^{i}$ | 0.1 (4) |
| C9—C4—C5—C6 | −178.4 (2) | | |

Symmetry code: (i) −*x*, −*y*+1, −*z*+2.

### *Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C1–C6 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8b···*Cg*1$^{ii}$ | 0.98 | 2.86 | 3.826 (3) | 171 |
| C10—H10a···*Cg*1$^{iii}$ | 0.95 | 2.98 | 3.788 (3) | 143 |

Symmetry codes: (ii) *x*, −*y*+1/2, *z*−1/2; (iii) *x*, −*y*+3/2, *z*+1/2.