

Bis(*p*-bromophenyl)dimethylsilane

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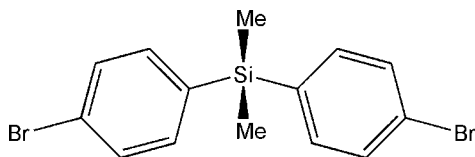
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.038; wR factor = 0.099; data-to-parameter ratio = 17.3.

The title compound, $\text{C}_{14}\text{H}_{14}\text{Br}_2\text{Si}$, has been used for more than 50 years as a synthon for the preparation of organosilicon polymers, but no structural data for this molecule have been available until now. The compound crystallizes with two crystallographically independent molecules in the asymmetric unit. In both molecules the Si atoms show tetrahedral coordination. The angles between the two benzene rings are $80.6(2)^\circ$ and $84.0(2)^\circ$.

Related literature

Bromophenyl-substituted organosilanes are of considerable interest for the preparation of organosilicon polymers (Speck, 1953; Ohshita *et al.*, 1994; Berger *et al.*, 1997; Kwak & Masuda, 2002*a,b*). These can be used as functionalized materials such as photoresists, precursors of ceramics, and conducting or photoconducting materials (Ohshita *et al.*, 1994). Furthermore, the title compound has been used as a synthon for the synthesis of the first silicon- and tin-containing paracyclophane (Zobel & Jurkschat, 1998). For related literature, see: Beyer *et al.* (2002); Doi *et al.* (1993); van Walree *et al.* (1995).



Experimental

Crystal data

| | |
|--|-----------------------------------|
| $\text{C}_{14}\text{H}_{14}\text{Br}_2\text{Si}$ | $V = 3053.11(12)$ Å ³ |
| $M_r = 370.16$ | $Z = 8$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation |
| $a = 12.4981(3)$ Å | $\mu = 5.37$ mm ⁻¹ |
| $b = 14.7956(3)$ Å | $T = 298(2)$ K |
| $c = 16.5144(4)$ Å | $0.35 \times 0.26 \times 0.22$ mm |
| $\beta = 91.208(1)^\circ$ | |

Data collection

| | |
|--|--|
| Bruker SMART CCD area-detector diffractometer | 53137 measured reflections |
| Absorption correction: multi-scan (SADABS; Sheldrick 1996) | 5380 independent reflections |
| $T_{\min} = 0.205$, $T_{\max} = 0.312$ | 4174 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.031$ |

Refinement

| | |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.038$ | 311 parameters |
| $wR(F^2) = 0.099$ | Only H-atom coordinates refined |
| $S = 1.07$ | $\Delta\rho_{\text{max}} = 0.66$ e Å ⁻³ |
| 5380 reflections | $\Delta\rho_{\text{min}} = -0.69$ e Å ⁻³ |

Table 1

Selected geometric parameters (Å, °).

| | | | |
|-----------|-----------|-------------|-----------|
| Si1—C2 | 1.852 (4) | Si2—C15 | 1.850 (4) |
| Si1—C1 | 1.858 (4) | Si2—C16 | 1.859 (4) |
| Si1—C9 | 1.873 (3) | Si2—C23 | 1.874 (3) |
| Si1—C3 | 1.877 (3) | Si2—C17 | 1.876 (3) |
| C2—Si1—C1 | 110.4 (2) | C15—Si2—C16 | 111.3 (2) |
| C2—Si1—C9 | 109.7 (2) | C15—Si2—C23 | 109.7 (2) |
| C1—Si1—C9 | 110.1 (2) | C16—Si2—C23 | 109.8 (2) |
| C2—Si1—C3 | 109.9 (2) | C15—Si2—C17 | 109.9 (2) |
| C1—Si1—C3 | 110.5 (2) | C16—Si2—C17 | 110.2 (2) |
| C9—Si1—C3 | 106.2 (1) | C23—Si2—C17 | 105.8 (1) |

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINTE* (Bruker, 2004); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2167).

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supplementary materials

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Bis(*p*-bromophenyl)dimethylsilane

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Comment

During our work on dipolar ferrocenylsilanes (Beyer *et al.*, 2002) we have prepared the title compound as a precursor for further syntheses. To our surprise, there were no structural data of the title compound available. The structure of bis(*p*-bromophenyl)dimethylsilicon has been determined to fill this gap.

Fig. 1 shows the molecular structure of the title compound and the atomic labelling scheme. It crystallizes with eight molecules in the unit cell. There are two crystallographically independent molecules in the asymmetric unit. Both silicon atoms are tetrahedrally coordinated. The angles between the benzene rings are contracted to 106.2 (1) (C9—Si1—C3) and 105.8 (1)° (C23—Si2—C17) respectively. The other bond angles at silicon are in the range 109.7 (2) to 111.3 (2)°. The Si—C bonds are in the typical range from 1.85 to 1.88 Å. The angles between the least-squares planes of the benzene rings are 80.6 (2)° for plane(C3—C8)-plane(C9—C14) and 84.0 (2)° for plane(C17—C22)-plane(C23—C28).

Experimental

The preparation of the title compound was performed according to methods described in the literature (Doi *et al.*, 1993; van Walree *et al.*, 1995) by reaction of *p*-dibromobenzene with *n*-butyllithium in diethyl ether followed by addition of dichlorodimethylsilane.

Refinement

Hydrogen atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å for Csp^2 and 0.96 for methyl. $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.2$ for Csp^2 and 1.5 for methyl.

Figures

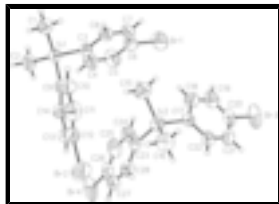


Fig. 1. The structure of the asymmetric unit of the title compound, drawn with 50% probability displacement ellipsoids.

bis(*p*-bromophenyl)dimethylsilane

Crystal data

C₁₄H₁₄Br₂Si

$F_{000} = 1456$

supplementary materials

$M_r = 370.16$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 12.4981 (3) \text{ \AA}$

$b = 14.7956 (3) \text{ \AA}$

$c = 16.5144 (4) \text{ \AA}$

$\beta = 91.208 (1)^\circ$

$V = 3053.11 (12) \text{ \AA}^3$

$Z = 8$

$D_x = 1.611 \text{ Mg m}^{-3}$

Melting point: 348 K

Mo $K\alpha$ radiation

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

Cell parameters from 6677 reflections

$\mu = 5.37 \text{ mm}^{-1}$

$T = 298 (2) \text{ K}$

Prism, colourless

$0.35 \times 0.26 \times 0.22 \text{ mm}$

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: sealed tube

Monochromator: graphite

$T = 298(2) \text{ K}$

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick 1996)

$T_{\min} = 0.205$, $T_{\max} = 0.312$

53137 measured reflections

5380 independent reflections

4174 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\max} = 25.0^\circ$

$\theta_{\min} = 1.9^\circ$

$h = -14 \rightarrow 14$

$k = -17 \rightarrow 17$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.099$

$S = 1.07$

5380 reflections

311 parameters

Primary atom site location: structure-invariant direct
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring
sites

Only H-atom coordinates refined

$$w = 1/[\sigma^2(F_o^2) + (0.0431P)^2 + 2.6376P]$$

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

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

$\Delta\rho_{\max} = 0.66 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.68 \text{ e \AA}^{-3}$

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 calculat-

ing 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 | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|-------------|--------------|----------------------------------|
| Si1 | 0.31077 (7) | 0.11971 (6) | 0.03855 (5) | 0.0470 (2) |
| Si2 | -0.02672 (7) | 0.37821 (6) | 0.19184 (5) | 0.0503 (2) |
| Br1 | 0.31205 (5) | 0.56124 (3) | 0.00621 (3) | 0.1027 (2) |
| Br2 | -0.08391 (4) | 0.06111 (4) | 0.28851 (4) | 0.0979 (2) |
| Br3 | -0.04008 (4) | 0.82134 (3) | 0.20446 (4) | 0.1059 (2) |
| Br4 | 0.28563 (6) | 0.30113 (4) | 0.50780 (4) | 0.1204 (3) |
| C1 | 0.2837 (3) | 0.0633 (3) | -0.0603 (2) | 0.0642 (9) |
| H1A | 0.3447 | 0.0698 | -0.0941 | 0.096* |
| H1B | 0.2224 | 0.0907 | -0.0863 | 0.096* |
| H1C | 0.2698 | 0.0003 | -0.0514 | 0.096* |
| C2 | 0.4368 (3) | 0.0766 (3) | 0.0852 (2) | 0.0669 (10) |
| H2A | 0.4959 | 0.0934 | 0.0522 | 0.100* |
| H2B | 0.4333 | 0.0119 | 0.0892 | 0.100* |
| H2C | 0.4464 | 0.1021 | 0.1383 | 0.100* |
| C3 | 0.3194 (2) | 0.2454 (2) | 0.02488 (18) | 0.0462 (7) |
| C4 | 0.3785 (3) | 0.2994 (3) | 0.0782 (3) | 0.0730 (11) |
| H4 | 0.4196 | 0.2721 | 0.1189 | 0.088* |
| C5 | 0.3781 (4) | 0.3925 (3) | 0.0726 (3) | 0.0812 (12) |
| H5 | 0.4188 | 0.4272 | 0.1087 | 0.097* |
| C6 | 0.3170 (3) | 0.4332 (2) | 0.0131 (2) | 0.0625 (9) |
| C7 | 0.2592 (3) | 0.3829 (2) | -0.0409 (2) | 0.0592 (9) |
| H7 | 0.2188 | 0.4109 | -0.0817 | 0.071* |
| C8 | 0.2608 (3) | 0.2907 (2) | -0.0350 (2) | 0.0546 (8) |
| H8 | 0.2211 | 0.2569 | -0.0724 | 0.066* |
| C9 | 0.1972 (3) | 0.0994 (2) | 0.10845 (19) | 0.0474 (7) |
| C10 | 0.0953 (3) | 0.0740 (3) | 0.0818 (2) | 0.0618 (9) |
| H10 | 0.0827 | 0.0643 | 0.0268 | 0.074* |
| C11 | 0.0122 (3) | 0.0627 (3) | 0.1347 (3) | 0.0684 (10) |
| H11 | -0.0554 | 0.0460 | 0.1153 | 0.082* |
| C12 | 0.0297 (3) | 0.0760 (2) | 0.2152 (2) | 0.0600 (9) |
| C13 | 0.1283 (3) | 0.1012 (3) | 0.2450 (2) | 0.0697 (10) |
| H13 | 0.1395 | 0.1105 | 0.3003 | 0.084* |
| C14 | 0.2106 (3) | 0.1125 (3) | 0.1917 (2) | 0.0617 (9) |
| H14 | 0.2776 | 0.1294 | 0.2119 | 0.074* |
| C15 | 0.0339 (4) | 0.3369 (3) | 0.0975 (2) | 0.0783 (12) |
| H15A | 0.0344 | 0.2720 | 0.0976 | 0.117* |
| H15B | 0.1059 | 0.3589 | 0.0944 | 0.117* |
| H15C | -0.0073 | 0.3582 | 0.0517 | 0.117* |
| C16 | -0.1616 (3) | 0.3284 (3) | 0.2059 (3) | 0.0719 (11) |
| H16A | -0.2079 | 0.3457 | 0.1615 | 0.108* |
| H16B | -0.1905 | 0.3502 | 0.2557 | 0.108* |
| H16C | -0.1560 | 0.2638 | 0.2079 | 0.108* |

supplementary materials

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|-----|-------------|------------|--------------|-------------|
| C17 | -0.0353 (3) | 0.5048 (2) | 0.18988 (19) | 0.0492 (7) |
| C18 | 0.0364 (3) | 0.5578 (3) | 0.1472 (3) | 0.0690 (10) |
| H18 | 0.0867 | 0.5294 | 0.1152 | 0.083* |
| C19 | 0.0354 (3) | 0.6508 (3) | 0.1507 (3) | 0.0762 (11) |
| H19 | 0.0844 | 0.6845 | 0.1217 | 0.091* |
| C20 | -0.0386 (3) | 0.6932 (2) | 0.1975 (3) | 0.0674 (11) |
| C21 | -0.1122 (3) | 0.6443 (3) | 0.2393 (2) | 0.0652 (10) |
| H21 | -0.1634 | 0.6734 | 0.2700 | 0.078* |
| C22 | -0.1093 (3) | 0.5517 (2) | 0.2355 (2) | 0.0578 (9) |
| H22 | -0.1590 | 0.5189 | 0.2646 | 0.069* |
| C23 | 0.0625 (3) | 0.3496 (2) | 0.2808 (2) | 0.0490 (8) |
| C24 | 0.1682 (3) | 0.3776 (3) | 0.2830 (2) | 0.0671 (10) |
| H24 | 0.1952 | 0.4073 | 0.2382 | 0.080* |
| C25 | 0.2352 (3) | 0.3630 (3) | 0.3493 (3) | 0.0783 (12) |
| H25 | 0.3060 | 0.3823 | 0.3493 | 0.094* |
| C26 | 0.1948 (4) | 0.3192 (3) | 0.4153 (3) | 0.0724 (12) |
| C27 | 0.0917 (4) | 0.2892 (3) | 0.4159 (2) | 0.0697 (11) |
| H27 | 0.0659 | 0.2588 | 0.4608 | 0.084* |
| C28 | 0.0265 (3) | 0.3045 (2) | 0.3493 (2) | 0.0602 (9) |
| H28 | -0.0439 | 0.2841 | 0.3498 | 0.072* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Si1 | 0.0492 (5) | 0.0458 (5) | 0.0459 (5) | 0.0050 (4) | -0.0004 (4) | 0.0006 (4) |
| Si2 | 0.0535 (5) | 0.0484 (5) | 0.0489 (5) | -0.0004 (4) | -0.0003 (4) | -0.0042 (4) |
| Br1 | 0.1552 (5) | 0.0477 (2) | 0.1055 (4) | -0.0094 (3) | 0.0104 (3) | 0.0062 (2) |
| Br2 | 0.0859 (3) | 0.0874 (3) | 0.1226 (4) | 0.0043 (2) | 0.0512 (3) | 0.0128 (3) |
| Br3 | 0.1000 (4) | 0.0501 (2) | 0.1655 (6) | 0.0063 (2) | -0.0449 (4) | -0.0005 (3) |
| Br4 | 0.1704 (6) | 0.0775 (3) | 0.1100 (4) | 0.0387 (3) | -0.0790 (4) | -0.0138 (3) |
| C1 | 0.079 (3) | 0.058 (2) | 0.056 (2) | -0.0001 (19) | 0.0043 (18) | -0.0061 (17) |
| C2 | 0.057 (2) | 0.068 (2) | 0.075 (2) | 0.0127 (18) | 0.0005 (18) | 0.011 (2) |
| C3 | 0.0475 (17) | 0.0485 (18) | 0.0425 (16) | 0.0016 (14) | 0.0011 (13) | -0.0006 (14) |
| C4 | 0.084 (3) | 0.060 (2) | 0.074 (3) | 0.000 (2) | -0.030 (2) | 0.000 (2) |
| C5 | 0.099 (3) | 0.059 (2) | 0.084 (3) | -0.014 (2) | -0.027 (2) | -0.010 (2) |
| C6 | 0.076 (2) | 0.0466 (19) | 0.066 (2) | -0.0037 (18) | 0.012 (2) | 0.0054 (17) |
| C7 | 0.072 (2) | 0.053 (2) | 0.052 (2) | 0.0019 (18) | -0.0023 (17) | 0.0105 (16) |
| C8 | 0.063 (2) | 0.053 (2) | 0.0478 (19) | -0.0013 (16) | -0.0057 (16) | -0.0006 (15) |
| C9 | 0.0509 (18) | 0.0404 (16) | 0.0510 (18) | 0.0064 (14) | -0.0016 (14) | 0.0000 (14) |
| C10 | 0.060 (2) | 0.069 (2) | 0.056 (2) | -0.0047 (18) | -0.0052 (17) | -0.0042 (18) |
| C11 | 0.051 (2) | 0.070 (3) | 0.084 (3) | -0.0063 (18) | -0.0017 (19) | 0.001 (2) |
| C12 | 0.057 (2) | 0.0478 (19) | 0.076 (3) | 0.0038 (16) | 0.0183 (18) | 0.0052 (18) |
| C13 | 0.075 (3) | 0.080 (3) | 0.055 (2) | 0.007 (2) | 0.0121 (19) | -0.003 (2) |
| C14 | 0.055 (2) | 0.075 (2) | 0.055 (2) | -0.0011 (18) | -0.0007 (16) | -0.0057 (18) |
| C15 | 0.094 (3) | 0.076 (3) | 0.065 (2) | 0.004 (2) | 0.010 (2) | -0.016 (2) |
| C16 | 0.061 (2) | 0.075 (3) | 0.079 (3) | -0.015 (2) | -0.0077 (19) | -0.006 (2) |
| C17 | 0.0486 (18) | 0.0526 (19) | 0.0459 (17) | 0.0021 (15) | -0.0067 (14) | 0.0031 (15) |
| C18 | 0.065 (2) | 0.061 (2) | 0.081 (3) | 0.0014 (19) | 0.013 (2) | 0.004 (2) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C19 | 0.073 (3) | 0.061 (2) | 0.095 (3) | -0.009 (2) | 0.001 (2) | 0.016 (2) |
| C20 | 0.067 (2) | 0.048 (2) | 0.086 (3) | 0.0087 (18) | -0.030 (2) | 0.0026 (19) |
| C21 | 0.063 (2) | 0.059 (2) | 0.073 (2) | 0.0178 (19) | -0.0074 (19) | -0.0067 (19) |
| C22 | 0.057 (2) | 0.060 (2) | 0.056 (2) | 0.0080 (17) | -0.0048 (16) | 0.0040 (17) |
| C23 | 0.0533 (19) | 0.0374 (16) | 0.0563 (19) | 0.0044 (14) | 0.0010 (15) | -0.0022 (14) |
| C24 | 0.060 (2) | 0.063 (2) | 0.078 (3) | -0.0062 (18) | -0.0039 (19) | 0.014 (2) |
| C25 | 0.067 (2) | 0.062 (2) | 0.106 (3) | -0.002 (2) | -0.023 (2) | 0.003 (2) |
| C26 | 0.094 (3) | 0.047 (2) | 0.075 (3) | 0.024 (2) | -0.029 (2) | -0.0076 (19) |
| C27 | 0.096 (3) | 0.054 (2) | 0.059 (2) | 0.017 (2) | 0.001 (2) | 0.0072 (18) |
| C28 | 0.063 (2) | 0.053 (2) | 0.065 (2) | 0.0066 (17) | 0.0064 (18) | 0.0007 (18) |

Geometric parameters (Å, °)

| | | | |
|-----------|-----------|-------------|-----------|
| Si1—C2 | 1.852 (4) | C11—C12 | 1.356 (6) |
| Si1—C1 | 1.858 (4) | C11—H11 | 0.9300 |
| Si1—C9 | 1.873 (3) | C12—C13 | 1.369 (6) |
| Si1—C3 | 1.877 (3) | C13—C14 | 1.379 (5) |
| Si2—C15 | 1.850 (4) | C13—H13 | 0.9300 |
| Si2—C16 | 1.859 (4) | C14—H14 | 0.9300 |
| Si2—C23 | 1.874 (3) | C15—H15A | 0.9600 |
| Si2—C17 | 1.876 (3) | C15—H15B | 0.9600 |
| Br1—C6 | 1.899 (4) | C15—H15C | 0.9600 |
| Br2—C12 | 1.899 (3) | C16—H16A | 0.9600 |
| Br3—C20 | 1.900 (4) | C16—H16B | 0.9600 |
| Br4—C26 | 1.903 (4) | C16—H16C | 0.9600 |
| C1—H1A | 0.9600 | C17—C22 | 1.390 (5) |
| C1—H1B | 0.9600 | C17—C18 | 1.394 (5) |
| C1—H1C | 0.9600 | C18—C19 | 1.378 (6) |
| C2—H2A | 0.9600 | C18—H18 | 0.9300 |
| C2—H2B | 0.9600 | C19—C20 | 1.369 (6) |
| C2—H2C | 0.9600 | C19—H19 | 0.9300 |
| C3—C8 | 1.389 (4) | C20—C21 | 1.369 (6) |
| C3—C4 | 1.390 (5) | C21—C22 | 1.372 (5) |
| C4—C5 | 1.380 (6) | C21—H21 | 0.9300 |
| C4—H4 | 0.9300 | C22—H22 | 0.9300 |
| C5—C6 | 1.371 (6) | C23—C24 | 1.384 (5) |
| C5—H5 | 0.9300 | C23—C28 | 1.397 (5) |
| C6—C7 | 1.357 (5) | C24—C25 | 1.381 (6) |
| C7—C8 | 1.368 (5) | C24—H24 | 0.9300 |
| C7—H7 | 0.9300 | C25—C26 | 1.373 (6) |
| C8—H8 | 0.9300 | C25—H25 | 0.9300 |
| C9—C10 | 1.390 (5) | C26—C27 | 1.363 (6) |
| C9—C14 | 1.394 (5) | C27—C28 | 1.374 (5) |
| C10—C11 | 1.381 (5) | C27—H27 | 0.9300 |
| C10—H10 | 0.9300 | C28—H28 | 0.9300 |
| C2—Si1—C1 | 110.4 (2) | C12—C13—C14 | 118.7 (4) |
| C2—Si1—C9 | 109.7 (2) | C12—C13—H13 | 120.6 |
| C1—Si1—C9 | 110.1 (2) | C14—C13—H13 | 120.6 |
| C2—Si1—C3 | 109.9 (2) | C13—C14—C9 | 122.5 (4) |

supplementary materials

| | | | |
|-------------|-----------|---------------|-----------|
| C1—Si1—C3 | 110.5 (2) | C13—C14—H14 | 118.8 |
| C9—Si1—C3 | 106.2 (1) | C9—C14—H14 | 118.8 |
| C15—Si2—C16 | 111.3 (2) | Si2—C15—H15A | 109.5 |
| C15—Si2—C23 | 109.7 (2) | Si2—C15—H15B | 109.5 |
| C16—Si2—C23 | 109.8 (2) | H15A—C15—H15B | 109.5 |
| C15—Si2—C17 | 109.9 (2) | Si2—C15—H15C | 109.5 |
| C16—Si2—C17 | 110.2 (2) | H15A—C15—H15C | 109.5 |
| C23—Si2—C17 | 105.8 (1) | H15B—C15—H15C | 109.5 |
| Si1—C1—H1A | 109.5 | Si2—C16—H16A | 109.5 |
| Si1—C1—H1B | 109.5 | Si2—C16—H16B | 109.5 |
| H1A—C1—H1B | 109.5 | H16A—C16—H16B | 109.5 |
| Si1—C1—H1C | 109.5 | Si2—C16—H16C | 109.5 |
| H1A—C1—H1C | 109.5 | H16A—C16—H16C | 109.5 |
| H1B—C1—H1C | 109.5 | H16B—C16—H16C | 109.5 |
| Si1—C2—H2A | 109.5 | C22—C17—C18 | 115.8 (3) |
| Si1—C2—H2B | 109.5 | C22—C17—Si2 | 121.8 (3) |
| H2A—C2—H2B | 109.5 | C18—C17—Si2 | 122.2 (3) |
| Si1—C2—H2C | 109.5 | C19—C18—C17 | 122.3 (4) |
| H2A—C2—H2C | 109.5 | C19—C18—H18 | 118.9 |
| H2B—C2—H2C | 109.5 | C17—C18—H18 | 118.9 |
| C8—C3—C4 | 116.0 (3) | C20—C19—C18 | 119.3 (4) |
| C8—C3—Si1 | 122.1 (2) | C20—C19—H19 | 120.4 |
| C4—C3—Si1 | 121.7 (3) | C18—C19—H19 | 120.4 |
| C5—C4—C3 | 122.0 (4) | C19—C20—C21 | 120.8 (4) |
| C5—C4—H4 | 119.0 | C19—C20—Br3 | 119.9 (3) |
| C3—C4—H4 | 119.0 | C21—C20—Br3 | 119.3 (3) |
| C6—C5—C4 | 119.2 (4) | C20—C21—C22 | 119.1 (4) |
| C6—C5—H5 | 120.4 | C20—C21—H21 | 120.5 |
| C4—C5—H5 | 120.4 | C22—C21—H21 | 120.5 |
| C7—C6—C5 | 120.7 (3) | C21—C22—C17 | 122.8 (4) |
| C7—C6—Br1 | 119.5 (3) | C21—C22—H22 | 118.6 |
| C5—C6—Br1 | 119.8 (3) | C17—C22—H22 | 118.6 |
| C6—C7—C8 | 119.5 (3) | C24—C23—C28 | 116.5 (3) |
| C6—C7—H7 | 120.2 | C24—C23—Si2 | 120.4 (3) |
| C8—C7—H7 | 120.2 | C28—C23—Si2 | 123.1 (3) |
| C7—C8—C3 | 122.6 (3) | C25—C24—C23 | 122.4 (4) |
| C7—C8—H8 | 118.7 | C25—C24—H24 | 118.8 |
| C3—C8—H8 | 118.7 | C23—C24—H24 | 118.8 |
| C10—C9—C14 | 116.1 (3) | C26—C25—C24 | 118.5 (4) |
| C10—C9—Si1 | 123.4 (3) | C26—C25—H25 | 120.8 |
| C14—C9—Si1 | 120.5 (3) | C24—C25—H25 | 120.8 |
| C11—C10—C9 | 121.9 (3) | C27—C26—C25 | 121.5 (4) |
| C11—C10—H10 | 119.0 | C27—C26—Br4 | 119.8 (4) |
| C9—C10—H10 | 119.0 | C25—C26—Br4 | 118.7 (4) |
| C12—C11—C10 | 119.6 (4) | C26—C27—C28 | 119.0 (4) |
| C12—C11—H11 | 120.2 | C26—C27—H27 | 120.5 |
| C10—C11—H11 | 120.2 | C28—C27—H27 | 120.5 |
| C11—C12—C13 | 121.2 (3) | C27—C28—C23 | 122.1 (4) |
| C11—C12—Br2 | 120.0 (3) | C27—C28—H28 | 119.0 |

| | | | |
|-----------------|------------|-----------------|------------|
| C13—C12—Br2 | 118.8 (3) | C23—C28—H28 | 119.0 |
| C2—Si1—C3—C8 | 153.4 (3) | C15—Si2—C17—C22 | 156.1 (3) |
| C1—Si1—C3—C8 | 31.3 (3) | C16—Si2—C17—C22 | 33.1 (3) |
| C9—Si1—C3—C8 | -88.0 (3) | C23—Si2—C17—C22 | -85.5 (3) |
| C2—Si1—C3—C4 | -31.8 (3) | C15—Si2—C17—C18 | -28.4 (4) |
| C1—Si1—C3—C4 | -153.9 (3) | C16—Si2—C17—C18 | -151.3 (3) |
| C9—Si1—C3—C4 | 86.8 (3) | C23—Si2—C17—C18 | 90.0 (3) |
| C8—C3—C4—C5 | 0.6 (6) | C22—C17—C18—C19 | 1.0 (6) |
| Si1—C3—C4—C5 | -174.5 (4) | Si2—C17—C18—C19 | -174.8 (3) |
| C3—C4—C5—C6 | 0.6 (7) | C17—C18—C19—C20 | -0.2 (7) |
| C4—C5—C6—C7 | -1.4 (7) | C18—C19—C20—C21 | -1.0 (6) |
| C4—C5—C6—Br1 | 178.2 (3) | C18—C19—C20—Br3 | 179.1 (3) |
| C5—C6—C7—C8 | 1.0 (6) | C19—C20—C21—C22 | 1.5 (6) |
| Br1—C6—C7—C8 | -178.6 (3) | Br3—C20—C21—C22 | -178.6 (3) |
| C6—C7—C8—C3 | 0.2 (6) | C20—C21—C22—C17 | -0.8 (6) |
| C4—C3—C8—C7 | -1.1 (5) | C18—C17—C22—C21 | -0.4 (5) |
| Si1—C3—C8—C7 | 174.0 (3) | Si2—C17—C22—C21 | 175.4 (3) |
| C2—Si1—C9—C10 | -141.8 (3) | C15—Si2—C23—C24 | 55.8 (3) |
| C1—Si1—C9—C10 | -20.1 (3) | C16—Si2—C23—C24 | 178.4 (3) |
| C3—Si1—C9—C10 | 99.4 (3) | C17—Si2—C23—C24 | -62.7 (3) |
| C2—Si1—C9—C14 | 40.4 (3) | C15—Si2—C23—C28 | -127.9 (3) |
| C1—Si1—C9—C14 | 162.0 (3) | C16—Si2—C23—C28 | -5.3 (3) |
| C3—Si1—C9—C14 | -78.4 (3) | C17—Si2—C23—C28 | 113.7 (3) |
| C14—C9—C10—C11 | 0.3 (5) | C28—C23—C24—C25 | -0.6 (6) |
| Si1—C9—C10—C11 | -177.6 (3) | Si2—C23—C24—C25 | 176.0 (3) |
| C9—C10—C11—C12 | -0.5 (6) | C23—C24—C25—C26 | -0.2 (6) |
| C10—C11—C12—C13 | 0.5 (6) | C24—C25—C26—C27 | 1.0 (6) |
| C10—C11—C12—Br2 | 179.8 (3) | C24—C25—C26—Br4 | -178.6 (3) |
| C11—C12—C13—C14 | -0.4 (6) | C25—C26—C27—C28 | -1.0 (6) |
| Br2—C12—C13—C14 | -179.6 (3) | Br4—C26—C27—C28 | 178.6 (3) |
| C12—C13—C14—C9 | 0.2 (6) | C26—C27—C28—C23 | 0.2 (5) |
| C10—C9—C14—C13 | -0.1 (5) | C24—C23—C28—C27 | 0.6 (5) |
| Si1—C9—C14—C13 | 177.9 (3) | Si2—C23—C28—C27 | -175.9 (3) |

Fig. 1

