Crystal structures of 2-bromo-1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilane and 2-bromo-1,1,1,3,3,3-hexaisopropyl-2-(triisopropylsilyl)-trisilane

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The synthesis and crystal structures of two tris(trialkylsilyl)silyl bromide compounds, C₉H₂₇BrSi₄ (I, HypSiBr) and C₂₇H₆₃BrSi₄ (II, TipSiBr), are described. Compound I was prepared in 85% yield by free-radical bromination of 1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilane using bromobutane and 2,2'-azobis(2-methylpropionitrile) as a radical initiator at 333 K. The molecule possesses threefold rotational symmetry, with the central Si atom and the Br atom being located on the threefold rotation axis. The Si—Br bond distance is 2.2990 (12) Å and the Si—Si bond lengths are 2.3477 (8) Å. The Br—Si—Si bond angles are 104.83 (3)/C₁₄ and the Si—Si—Si bond angles are 113.69 (2)/C₁₄, reflecting the steric hindrance inherent in the three trimethylsilyl groups attached to the central Si atom. Compound II was prepared in 55% yield by free-radical bromination of 1,1,1,3,3,3-hexaisopropyl-2-(triisopropylsilyl)trisilane using N-bromosuccinimide and 2,2'-azobis(2-methylpropionitrile) as a radical initiator at 333 K. Here the Si—Br bond length is 2.3185 (7) Å and the Si—Si bond angles range from 104.83 (3)/C₁₄ to 103.77 (3)/C₁₄, indicating steric hindrance between the three triisopropylsilyl groups.

1. Chemical context

The steric and electronic effects of the tris(trimethylsilyl)silyl group have been exploited for the synthesis and study of a variety of reactive centers including silylenes (Wendel et al., 2017) and silylanions (Kayser et al., 2002; Mechtler et al., 2004; Zirngast et al., 2008; Marschner, 2015). This sterically hindered group has been shown to lead to lower coordination by solvent when it is attached to organolithium compounds (Feil & Harder, 2003). It has also been used in organic synthesis to produce highly stereoselective aldol reactions leading to unique reactivity (Gati & Yamamoto, 2016). For this research we prepared tris(trimethylsilyl)silylv bromide (HypSiBr) as a precursor to vinyltris(trimethylsilyl)silane. The even bulkier tris(triisopropylsilyl)silylv bromide (TipSiBr) was prepared as a potential precursor to methoxytris(triisopropylsilyl)silane. Herein, we report on the crystal structures of these two sterically hindered silyl bromides 2-bromo-1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilane (I), and 2-bromo-1,1,1,3,3,3-hexaisopropyl-2-(triisopropylsilyl)-trisilane (II).
2. Structural commentary

The molecular structure of compound I (HypSiBr), is shown in Fig. 1, and selected geometrical parameters are given in Table 1. The asymmetric unit is composed of one trimethylsilyl group, with the central silicon atom Si1 and the bromine atom Br1 lying on a threefold rotation axis. This supersilylbromide crystallized in the cubic space group \(Pa\bar{3}\) with a central four-coordinate silicon atom, Si1, that deviates slightly from an ideal tetrahedron due to the steric bulk of the attached trimethylsilyl (TMS) groups. The \(\tau_4\) descriptor for fourfold coordination around Si1 is 0.94 (where, for extreme forms, \(\tau_4\) = 0.00 for square-planar, 1.00 for tetrahedral and 0.85 for trigonal–pyramidal; Yang et al., 2007). Interestingly, the \(\tau_4\) descriptor values for atoms Si2, Si3 and Si4 (the silicon atoms of the triisopropylsilyl groups) are 0.96, 0.97 and 0.95, respectively, indicating that their coordination geometry is closest to an ideal tetrahedron.

3. Supramolecular features

There are no significant intermolecular contacts, other than weak van der Waals interactions, present in the crystals of compounds I or II. Compound II, however, contains four intramolecular C–H···Br hydrogen bonds (Table 2, Fig. 3). These hydrogen bonds contain \(D···A\) distances that range indicating that the trimethylsilyl groups are forced away from one another. The Si1–Br1 bond length is 2.2990 (12) Å. As for Si2, the C–Si2–C bond angles range from 107.1 (2) to 110.55 (17), while the C–Si2–Si1 bond angles range from 108.61 (10) to 110.16 (11).

The asymmetric unit of compound II (TipSiBr), is shown in Fig. 2, and selected geometrical parameters are given in Table 1. This compound crystallized in the triclinic space group \(Pt\bar{1}\) with a central four-coordinate silicon atom, Si1, that deviates from the ideal tetrahedron as shown from its \(\tau_4\) descriptor for fourfold coordination of 0.90. The Br1–Si1–Si2/Si3/Si4 bond angles range from 98.44 (3) to 103.77 (3), and the Si1–Br1 bond distance is 2.3185 (7) Å, which is longer than that of compound I [2.2990 (12) Å]. The \(\tau_4\) descriptor values for atoms Si2, Si3 and Si4 (the silicon atoms of the triisopropylsilyl groups) are 0.96, 0.97 and 0.95, respectively, indicating that their coordination geometry is closest to an ideal tetrahedron.
angles that range from 131 to 155°.

4. Database survey

The Cambridge Structural Database (CSD, version 5.39, February 2018; Groom et al., 2016) contains 1398 structures containing a SiSi group. Of these, there are only 42 structures where the central silicon atom is bonded directly to a halogen.

Of particular interest to this work is the structure of tris(trimethylsilyl)chlorosilane (III, HypSiCl) [CSD refcode QULWEA; Kuzora et al., 2009], the isotypic chloro derivative of compound I, and the structure of (iPr3Si)3SiH (IV, TipSiH), isotypic with compounds I and III. The analysis of IV by both X-ray and neutron diffraction has been described by Gaspar et al. (1999). Table 1 contains pertinent bond lengths and bond angles for compounds I, II, III (HypSiCl) and IV (TipSiH).

For compounds I and III the Si—X bond lengths follow the expected trend with the Si1—Cl bond length of QULWEA at 2.1248 (9) Å compared to the Si1—Br1 bond length of 2.2990 (12) Å for compound I. The Si1—Si2 bond length of the bromo derivative I reported here is 2.3477 (8) Å, which is slightly longer than the Si1—Si2 bond length of the chloro derivative at 2.3406 (6) Å. The central silicon atom of the chloro derivative appears less sterically hindered with an Si2—Si1—Cl bond angle of 115.02 (4)° and Si2—Si1—Si2i,ii bond angles of 113.126 (4)° versus a smaller Si2—Si1—Br1 bond angle of 104.83 (3)° and a larger Si2—Si1—Si2i,ii bond angle of 136.69 (2)° for compound I [symmetry codes: (i) z, x, y; (ii) y, z, x]. The protio derivative (HypSiH) is a liquid at room temperature, and the structure of the iodo derivative (HypSiI) has not been deposited in the CSD.

The X-ray data for compound IV (TipSiH) was not found in the CSD, but the journal article (Gaspar et al., 1999) contains all pertinent structural data to allow for a comparison with (iPr3Si)3SiBr, viz. compound II (TipSiBr). Like compounds I and III, compound IV crystallizes in the cubic space group Pa3, and the molecule possesses threefold rotation symmetry.

The presence of a small hydrogen atom bonded to the central silicon atom Si1 allows the three (iPr3Si) groups to push further away from one another, resulting in Si2—Si1—Si2i,ii bond angles of 117.9 (1)° and Si2—Si1—H bond angles of 98.3 (1)° [symmetry codes: (i) z, x, y; (ii) y, z, x]. In II, the corresponding Si—Si—Br bond angles range from 115.02 (4)° to 116.59 (4)° and the Si—Si—Br bond angles vary from 98.44 (3)° to 103.77 (3)°.

5. Synthesis and crystallization

**Compound I**: Tris(trimethylsilylsilyl)silane (2.0 g, 8.0 mmol) was added to an oven-dried nitrogen-flushed 250 ml Schlenk flask with a stir-bar. Bromobutane (2.0 g, 14.6 mmol) was filtered through a plug of silica gel in a Pasteur pipette and was transferred into the Schlenk flask. AIBN [2,2-azobis(2-methylpropionitrile); 20 mg] was then added to the flask, and the reaction was heated to 333 K using an oil bath and then

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**Table 1**

| Compound | I (HypSiBr) | II (TipSiBr) | III (HypSiCl) | IV (TipSiH) |
|----------|-------------|--------------|---------------|-------------|
| Si1—Xd   | 2.2990 (12) | 2.3185 (7)   | 2.1248 (9)    | 1.608 (1)   |
| Si1—Si0  | 2.3477 (8)  | 2.4430 (10), 2.4448 (10), 2.4628 (9) | 2.3406 (6) | 2.405 (1) |
| Si2—Si1—Si2 i,ii | 113.69 (2) | 115.02 (4), 116.55 (3), 116.59 (4) | 113.13 (2) | 117.9 (1) |
| Si2—X0   | 104.83 (3)  | 98.44 (3) to 103.77 (3) | 105.51 (2) | 98.3 (1) |
| τ of Si1 | 0.94        | 0.90         | 0.95          | 0.88        |

**Table 2**

Hydrogen-bond geometry (Å, °) for II.

| D—H···A | H···A | D—H···A | D—H···A |
|---------|-------|---------|---------|
| C5—H5B···Br1 | 0.98 | 2.80 | 3.711 (3) | 155 |
| C16—H16···Br1 | 1.00 | 2.84 | 3.584 (3) | 131 |
| C23—H23A···Br1 | 0.98 | 2.87 | 3.685 (3) | 142 |
| C24—H24C···Br1 | 0.98 | 2.93 | 3.726 (3) | 139 |

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**Figure 3**

Intramolecular C—H···Br hydrogen bonds (blue dashed lines; see Table 2) present in compound II. For clarity, only the hydrogen atoms involved in a hydrogen bonding are shown.
heating was stopped. After stirring the reaction overnight at room temperature, GC–MS analysis of a sample indicated incomplete reaction and more AIBN (11 mg) was added to the flask. The reaction was heated once more to 333 K for 1 h. Analysis by GC–MS now indicated that the reaction was complete. The flask was placed in a freezer at 243 K and left for 16 h. Removal of the solvent in vacuo yielded 2.2 g (85%). 1H NMR (300 MHz, C 6D6) δ 0.01 (s, 42H), 0.47 (s, 7H); 13C NMR (75 MHz, chloroform-d) δ 33.6, 42.1, 110.8 ppm; GC–MS: 11.24 min, base peak: 73.

**Compound II**: Tris(triisopropylsilyl)silane (110 mg, 0.22 mmol) was dissolved in freshly distilled benzene (10 ml) along with NBS (45 mg) and AIBN (2 mg, initiator). The mixture was heated using an oil bath at 333 K for 30 min, when GC–MS analysis indicated that no reaction had occurred. At this point the solution was heated with a heat gun until the reaction mixture turned slightly yellow. The yellow colour dissipated in less than 1 min. Analysis of the reaction mixture by 1H NMR indicated that only 60% of the starting material had been consumed. An additional amount of NBS (N-bromosuccinimide; 20 mg) was added to the reaction flask, and the solution was again heated with a heat gun. The product was isolated by removing the solvent in vacuo and extracting the product from the crude reaction mixture with pentane. The pentane solution was filtered through glass wool, concentrated and weighed (135 mg). Analysis of the product with 1H NMR indicated this was 90% pure. The product was further purified by dissolving this solid in 1 ml pentane, cooling to 195 K and isolating the colourless needle-like crystals of II by removing the solvent with a syringe, washing with pentane and drying in vacuo (yield 62 mg, 55%). 1H NMR (300 MHz, C 6D6) δ 1.34 (d, J = 7.3 Hz, 54H), 1.66 (heptet, J = 7.4 Hz, 9H); 13C NMR (75 MHz, chloroform-d) δ 16.4, 21.6; HRMS for C27H63BrSi4 calculated 535.2642 (M – C3H5), found 535.2641.

### 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. For both compounds the hydrogen atoms were placed in calculated positions and refined using a riding model: C—H = 0.98-1.00 Å with eq(C) for other H atoms.

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Crystal structures of 2-bromo-1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilane and 2-bromo-1,1,1,3,3,3-hexaisopropyl-2-(triisopropylsilyl)trisilane

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Computing details

Data collection: *APEX2* (Bruker, 2014) for (I); *SMART* (Bruker, 2014) for (II). For both structures, cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014). Program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008) for (I); *SHELXT2013* (Sheldrick, 2015a) for (II). Program(s) used to refine structure: *SHELXL2017* (Sheldrick, 2015b) for (I); *SHELXL2014* (Sheldrick, 2015b) for (II). Molecular graphics: *OLEX2* (Dolomanov et al., 2009; Bourhis et al., 2015) for (I); *SHELXTL* (Sheldrick, 2008) for (II). Software used to prepare material for publication: *CrystalMaker* (Palmer, 2007) for (I); *SHELXTL* (Sheldrick, 2008) for (II).

2-Bromo-1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilane (I)

Crystal data

\[ \text{C}_9\text{H}_{27}\text{BrSi}_4 \]

\( M_r = 327.57 \)

Cubic, \( Pa\bar{3} \)

\( a = 15.6497 \) (19) Å

\( V = 3832.8 \) (14) Å\(^3\)

\( Z = 8 \)

\( F(000) = 1376 \)

\( D_x = 1.135 \text{ Mg m}^{-3} \)

Mo \( K\alpha \) radiation, \( \lambda = 0.71073 \) Å

Cell parameters from 3863 reflections

\( \theta = 2.3-25.3^\circ \)

\( \mu = 2.37 \text{ mm}^{-1} \)

\( T = 173 \text{ K} \)

Block, colourless

\( 0.45 \times 0.24 \times 0.14 \text{ mm} \)

Data collection

Bruker APEXII CCD

diffractometer

\( \varphi \) and \( \omega \) scans

Absorption correction: multi-scan

(SADABS; Bruker, 2014)

\( T_{\text{min}} = 0.571, T_{\text{max}} = 0.745 \)

11038 measured reflections

1174 independent reflections

953 reflections with \( I > 2\sigma(I) \)

\( R_{\text{int}} = 0.046 \)

\( \theta_{\text{max}} = 25.3^\circ, \theta_{\text{min}} = 2.3^\circ \)

\( h = -18 \rightarrow 16 \)

\( k = -18 \rightarrow 17 \)

\( l = -15 \rightarrow 18 \)

Refinement

Refinement on \( F^2 \)

Least-squares matrix: full

\( R[F^2 > 2\sigma(F^2)] = 0.028 \)

\( wR(F^2) = 0.075 \)

\( S = 1.05 \)

1174 reflections

46 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
\[ w = \frac{1}{[\sigma^2(F_o^2) + (0.0349P)^2 + 1.4333P]} \]

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

(\(\Delta/\sigma\))_{max} = 0.002

\(\Delta\rho_{max} = 0.31 \text{ e Å}^{-3}\)

\(\Delta\rho_{min} = -0.16 \text{ e Å}^{-3}\)

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.

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

|     | x          | y          | z          | U_{iso} or U_{eq} |
|-----|------------|------------|------------|-------------------|
| Br1 | 0.74011 (2) | 0.74011 (2)| 0.74011 (2)| 0.04337 (17)      |
| Si1 | 0.65529 (4) | 0.65529 (4)| 0.65529 (4)| 0.0327 (3)        |
| Si2 | 0.69238 (5) | 0.51472 (4)| 0.69229 (5)| 0.0473 (2)        |
| C1  | 0.6249 (2)  | 0.43945 (18)| 0.6286 (2) | 0.0734 (10)       |
| H1A | 0.6331      | 0.4506     | 0.5675     | 0.110*            |
| H1B | 0.5646      | 0.4478     | 0.6434     | 0.110*            |
| H1C | 0.6415      | 0.3805     | 0.6414     | 0.110*            |
| C2  | 0.8079 (2)  | 0.49575 (19)| 0.6707 (3) | 0.0943 (14)       |
| H2A | 0.8227      | 0.4370     | 0.6866     | 0.141*            |
| H2B | 0.8422      | 0.5358     | 0.7044     | 0.141*            |
| H2C | 0.8194      | 0.5044     | 0.6098     | 0.141*            |
| C3  | 0.6752 (3)  | 0.49746 (19)| 0.8090 (2) | 0.0953 (13)       |
| H3A | 0.6142      | 0.5032     | 0.8222     | 0.143*            |
| H3B | 0.7076      | 0.5401     | 0.8414     | 0.143*            |
| H3C | 0.6946      | 0.4401     | 0.8247     | 0.143*            |

**Atomic displacement parameters (Å²)**

|      | U₁₁     | U₂₂     | U₃₃     | U₁₂    | U₁₃    | U₂₃    |
|------|---------|---------|---------|--------|--------|--------|
| Br1  | 0.04337 (17) | 0.04337 (17) | 0.04337 (17) | -0.00621 (10) | -0.00621 (10) | -0.00621 (10) |
| Si1  | 0.0327 (3)    | 0.0327 (3)    | 0.0327 (3)    | -0.0008 (3)    | -0.0008 (3)    | -0.0008 (3)    |
| Si2  | 0.0529 (5)    | 0.0317 (4)    | 0.0573 (5)    | -0.0013 (3)    | -0.0106 (4)    | 0.0008 (3)     |
| C1   | 0.087 (2)     | 0.0426 (16)   | 0.091 (2)     | -0.0092 (16)   | -0.0304 (19)   | -0.0051 (16)   |
| C2   | 0.056 (2)     | 0.0494 (19)   | 0.178 (4)     | 0.0145 (16)    | -0.007 (2)     | 0.001 (2)      |
| C3   | 0.168 (4)     | 0.052 (2)     | 0.066 (2)     | 0.006 (2)      | -0.019 (2)     | 0.0183 (17)    |

**Geometric parameters (Å, °)**

|      | Br1—Si1   | 2.2990 (12) | Si2—C1   | 1.870 (3)   |
|------|-----------|-------------|----------|-------------|
| Si1—Si2 | 2.3478 (8) | Si2—C2    | 1.862 (3) |
| Si1—Si2 | 2.3477 (8) | Si2—C3    | 1.866 (3) |
| Si1—Si2 ii | 2.3478 (8) |          |          |             |
| Br1—Si1—Si2 | 104.83 (3) | C1—Si2—Si1 | 108.61 (10) |
| Br1—Si1—Si2 ii | 104.83 (3) | C2—Si2—Si1 | 110.16 (11) |
| Br1—Si1—Si2 i | 104.83 (3) | C2—Si2—C1 | 110.55 (17) |

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Supporting information

2-Bromo-1,1,1,3,3,3-hexaisopropyl-2-(triisopropylsilyl)trisilane (II)

Crystal data

C_{27}H_{63}BrSi_{4}

Mr = 580.04

Triclinic, P1

a = 8.4412 (4) Å

b = 11.1336 (6) Å

c = 18.8477 (10) Å

α = 92.565 (4)°

β = 90.527 (4)°

γ = 108.718 (4)°

V = 1675.44 (15) Å³

Z = 2

F(000) = 632

D_x = 1.150 Mg m⁻³

Mo Kα radiation, λ = 0.71073 Å

Cell parameters from 8192 reflections

θ = 2.0–26.0°

µ = 1.38 mm⁻¹

T = 173 K

Needles, colourless

V = 1675.44 (15) Å³

0.38 × 0.10 × 0.02 mm

Data collection

Bruker SMART APEX CCD area detector diffractometer

Radiation source: sealed tube

Detector resolution: 8 pixels mm⁻¹

ω and φ scans

Absorption correction: multi-scan

(TADABS; Bruker, 2014)

T_min = 0.554, T_max = 0.674

21505 measured reflections

6628 independent reflections

4752 reflections with I > 2σ(I)

R(int) = 0.057

θ_max = 26.3°, θ_min = 1.1°

h = −10→10

k = −13→13

l = −23→23

Refinement

Refinement on F²

Least-squares matrix: full

R[F² > 2σ(F²)] = 0.037

wR(F²) = 0.075

S = 1.01

6628 reflections

307 parameters

0 restraints

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

w = 1/[σ²(F_c) + (0.0274P)² + 0.3128P]

where P = (F_c² + 2F_o²)/3

H atoms: C—H = 0.95–0.99 Å and wAith U_iso(H) = 1.2 (1.5 for methyl groups) times U_eq(C)

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. All H atoms were positioned geometrically and refined using a riding model with C—H = 0.95–0.99 Å and wAith U_iso(H) = 1.2 (1.5 for methyl groups) times U_eq(C).

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

| Atom | x       | y       | z       | U_iso(eq)/U_eq |
|------|---------|---------|---------|---------------|
| Br1  | 1.06221 (3) | 0.19737 (3) | 0.24790 (2) | 0.02768 (9) |
| Atom | X        | Y        | Z        | U11    |
|------|----------|----------|----------|--------|
| Si1  | 0.77723  | 0.16573  | 0.25116  | 0.01926|
| Si2  | 0.72101  | 0.26469  | 0.14487  | 0.02137|
| Si3  | 0.67829  | -0.06634 | 0.24791  | 0.02310|
| Si4  | 0.74993  | 0.27556  | 0.36447  | 0.02177|
| C1   | 0.8269   | 0.4443   | 0.15761  | 0.02490|
| H1   | 0.7549   | 0.4757   | 0.1905   | 0.030  |
| C2   | 1.0018   | 0.4866   | 0.19270  | 0.03490|
| H2A  | 1.0777   | 0.4575   | 0.1626   | 0.052  |
| H2B  | 0.9962   | 0.4498   | 0.2393   | 0.052  |
| H2C  | 1.0435   | 0.5794   | 0.1987   | 0.052  |
| C3   | 0.8371   | 0.5176   | 0.08928  | 0.03350|
| H3A  | 0.8753   | 0.6091   | 0.1015   | 0.050  |
| H3B  | 0.7262   | 0.4931   | 0.0660   | 0.050  |
| H3C  | 0.9162   | 0.4972   | 0.0570   | 0.050  |
| C4   | 0.7935   | 0.1980   | 0.06084  | 0.02660|
| H4   | 0.7464   | 0.1034   | 0.0618   | 0.032  |
| C5   | 0.9832   | 0.2301   | 0.05683  | 0.03710|
| H5A  | 1.0101   | 0.1830   | 0.0161   | 0.056  |
| H5B  | 1.0268   | 0.2065   | 0.1006   | 0.056  |
| H5C  | 1.0345   | 0.3214   | 0.0513   | 0.056  |
| C6   | 0.7282   | 0.2347   | -0.00855 | 0.03880|
| H6A  | 0.7814   | 0.3257   | -0.0146  | 0.058  |
| H6B  | 0.6067   | 0.2155   | -0.0066  | 0.058  |
| H6C  | 0.7549   | 0.1862   | -0.0487  | 0.058  |
| C7   | 0.4836   | 0.2270   | 0.13810  | 0.02870|
| H7   | 0.4439   | 0.2136   | 0.1879   | 0.034  |
| C8   | 0.4264   | 0.3368   | 0.11280  | 0.04290|
| H8A  | 0.4536   | 0.3500   | 0.0627   | 0.064  |
| H8B  | 0.4841   | 0.4146   | 0.1414   | 0.064  |
| H8C  | 0.3053   | 0.3155   | 0.1182   | 0.064  |
| C9   | 0.3878   | 0.1029   | 0.09537  | 0.03940|
| H9A  | 0.2692   | 0.0772   | 0.1073   | 0.059  |
| H9B  | 0.4342   | 0.0360   | 0.1073   | 0.059  |
| H9C  | 0.3991   | 0.1169   | 0.0444   | 0.059  |
| C10  | 0.6700   | -0.1257  | 0.15145  | 0.03040|
| H10  | 0.6105   | -0.0769  | 0.1245   | 0.036  |
| C11  | 0.8446   | -0.0949  | 0.11986  | 0.04020|
| H11A | 0.9038   | -0.1481  | 0.1406   | 0.060  |
| H11B | 0.9078   | -0.0052  | 0.1305   | 0.060  |
| H11C | 0.8337   | -0.1118  | 0.0683   | 0.060  |
| C12  | 0.5697   | -0.2671  | 0.13666  | 0.04230|
| H12A | 0.5798   | -0.2910  | 0.0866   | 0.063  |
| H12B | 0.4517   | -0.2814  | 0.1470   | 0.063  |
| H12C | 0.6138   | -0.3189  | 0.1669   | 0.063  |
| C13  | 0.4641   | -0.1251  | 0.28895  | 0.02780|
| H13  | 0.4741   | -0.0754  | 0.3352   | 0.033  |
| C14  | 0.3289   | -0.0951  | 0.24525  | 0.04260|
| H14A | 0.3107   | -0.1440  | 0.1997   | 0.064  |
| Atom  | x       | y       | z       | Ueq   |
|-------|---------|---------|---------|-------|
| H14B  | 0.3651  | -0.0041 | 0.2367  | 0.064*|
| H14C  | 0.2244  | -0.1178 | 0.2714  | 0.064*|
| C15   | 0.4016  | -0.2660 | 0.30713 | 0.0402|
| H15A  | 0.2967  | -0.2836 | 0.3327  | 0.060*|
| H15B  | 0.4859  | -0.2842 | 0.3371  | 0.060*|
| H15C  | 0.3827  | -0.3196 | 0.2632  | 0.060*|
| C16   | 0.8392  | -0.1171 | 0.29934 | 0.0292|
| H16   | 0.9513  | -0.0608 | 0.2850  | 0.035*|
| C17   | 0.8383  | -0.2537 | 0.28398 | 0.0383|
| H17A  | 0.9229  | -0.2705 | 0.3143  | 0.057*|
| H17B  | 0.8637  | -0.2649 | 0.2340  | 0.057*|
| H17C  | 0.7277  | -0.3129 | 0.2938  | 0.057*|
| C18   | 0.8317  | -0.0933 | 0.38032 | 0.0461|
| H18A  | 0.7258  | -0.1494 | 0.3976  | 0.069*|
| H18B  | 0.8392  | -0.0047 | 0.3909  | 0.069*|
| H18C  | 0.9252  | -0.1109 | 0.4039  | 0.069*|
| C19   | 0.5967  | 0.1584  | 0.42272 | 0.0290|
| H19   | 0.6217  | 0.0766  | 0.4166  | 0.035*|
| C20   | 0.4130  | 0.1287  | 0.40018 | 0.0467|
| H20A  | 0.3450  | 0.0522  | 0.4228  | 0.070*|
| H20B  | 0.4012  | 0.1145  | 0.3484  | 0.070*|
| H20C  | 0.3751  | 0.2003  | 0.4149  | 0.070*|
| C21   | 0.6171  | 0.1952  | 0.50277 | 0.0486|
| H21A  | 0.5929  | 0.2749  | 0.5118  | 0.073*|
| H21B  | 0.7321  | 0.2064  | 0.5185  | 0.073*|
| H21C  | 0.5392  | 0.1280  | 0.5290  | 0.073*|
| C22   | 0.9557  | 0.3395  | 0.41777 | 0.0286|
| H22   | 0.9246  | 0.3756  | 0.4631  | 0.034*|
| C23   | 1.0335  | 0.2414  | 0.44175 | 0.0397|
| H23A  | 1.0703  | 0.2024  | 0.4002  | 0.059*|
| H23B  | 0.9504  | 0.1757  | 0.4669  | 0.059*|
| H23C  | 1.1299  | 0.2831  | 0.4736  | 0.059*|
| C24   | 1.0893  | 0.4526  | 0.38677 | 0.0364|
| H24A  | 1.1806  | 0.4887  | 0.4218  | 0.055*|
| H24B  | 1.0390  | 0.5175  | 0.3750  | 0.055*|
| H24C  | 1.1334  | 0.4236  | 0.3437  | 0.055*|
| C25   | 0.6831  | 0.4212  | 0.34999 | 0.0258|
| H25   | 0.7695  | 0.4766  | 0.3192  | 0.031*|
| C26   | 0.6873  | 0.5007  | 0.41963 | 0.0450|
| H26A  | 0.6597  | 0.5772  | 0.4092  | 0.067*|
| H26B  | 0.7994  | 0.5251  | 0.4417  | 0.067*|
| H26C  | 0.6053  | 0.4502  | 0.4522  | 0.067*|
| C27   | 0.5152  | 0.3988  | 0.31189 | 0.0392|
| H27A  | 0.4243  | 0.3572  | 0.3434  | 0.059*|
| H27B  | 0.5082  | 0.3445  | 0.2688  | 0.059*|
| H27C  | 0.5050  | 0.4803  | 0.2990  | 0.059*|

*Estimated standard deviation.
### Atomic displacement parameters (Å$^2$)

|    | $U^{11}$   | $U^{22}$   | $U^{33}$   | $U^{12}$   | $U^{13}$   | $U^{23}$   |
|----|------------|------------|------------|------------|------------|------------|
| Br1 | 0.02088 (14) | 0.03279 (18) | 0.02927 (15) | 0.00846 (11) | 0.00155 (11) | 0.00149 (12) |
| Si1 | 0.0195 (4) | 0.0190 (4) | 0.0191 (4) | 0.0060 (3) | 0.0012 (3) | 0.0007 (3) |
| Si2 | 0.0215 (4) | 0.0220 (4) | 0.0204 (4) | 0.0066 (3) | 0.0003 (3) | 0.0017 (3) |
| Si3 | 0.0256 (4) | 0.0192 (4) | 0.0247 (4) | 0.0076 (3) | 0.0019 (3) | 0.0009 (3) |
| Si4 | 0.0255 (4) | 0.0205 (4) | 0.0195 (4) | 0.0075 (3) | 0.0028 (3) | 0.0008 (3) |
| C1  | 0.0272 (14) | 0.0233 (15) | 0.0229 (14) | 0.0060 (12) | 0.0038 (11) | 0.0043 (11) |
| C2  | 0.0326 (16) | 0.0281 (17) | 0.0391 (17) | 0.0031 (13) | −0.0053 (13) | 0.0016 (13) |
| C3  | 0.0416 (18) | 0.0255 (16) | 0.0336 (16) | 0.0103 (13) | 0.0054 (13) | 0.0078 (13) |
| C4  | 0.0325 (15) | 0.0280 (16) | 0.0199 (13) | 0.0110 (12) | −0.0005 (11) | −0.0002 (11) |
| C5  | 0.0398 (18) | 0.049 (2) | 0.0266 (15) | 0.0205 (15) | 0.0080 (13) | 0.0018 (14) |
| C6  | 0.0447 (18) | 0.047 (2) | 0.0228 (15) | 0.0122 (15) | −0.0018 (13) | −0.0007 (14) |
| C7  | 0.0234 (15) | 0.0325 (17) | 0.0306 (15) | 0.0091 (12) | −0.0023 (12) | 0.0033 (13) |
| C8  | 0.0280 (16) | 0.044 (2) | 0.059 (2) | 0.0136 (14) | −0.0057 (15) | 0.0083 (16) |
| C9  | 0.0287 (16) | 0.0406 (19) | 0.0425 (18) | 0.0022 (14) | −0.0059 (13) | 0.0037 (14) |
| C10 | 0.0392 (17) | 0.0255 (16) | 0.0284 (15) | 0.0138 (13) | 0.0009 (13) | −0.0026 (12) |
| C11 | 0.053 (2) | 0.0409 (19) | 0.0339 (16) | 0.0245 (15) | 0.0101 (15) | 0.0006 (14) |
| C12 | 0.055 (2) | 0.0358 (19) | 0.0371 (17) | 0.0182 (16) | −0.0091 (15) | −0.0096 (14) |
| C13 | 0.0281 (15) | 0.0207 (15) | 0.0328 (15) | 0.0053 (12) | 0.0030 (12) | 0.0029 (12) |
| C14 | 0.0303 (17) | 0.044 (2) | 0.052 (2) | 0.0098 (14) | 0.0021 (14) | 0.0088 (15) |
| C15 | 0.0404 (18) | 0.0301 (17) | 0.0447 (18) | 0.0030 (14) | 0.0061 (14) | 0.0067 (14) |
| C16 | 0.0312 (15) | 0.0220 (16) | 0.0371 (16) | 0.0119 (12) | −0.0010 (12) | 0.0045 (12) |
| C17 | 0.0431 (18) | 0.0310 (18) | 0.0456 (18) | 0.0180 (14) | 0.0007 (15) | 0.0072 (14) |
| C18 | 0.062 (2) | 0.042 (2) | 0.0410 (18) | 0.0268 (17) | −0.0133 (16) | −0.0041 (15) |
| C19 | 0.0364 (16) | 0.0218 (16) | 0.0287 (15) | 0.0086 (12) | 0.0091 (12) | 0.0038 (12) |
| C20 | 0.0369 (18) | 0.0338 (19) | 0.069 (2) | 0.0089 (14) | 0.0210 (16) | 0.0101 (16) |
| C21 | 0.075 (2) | 0.036 (2) | 0.0324 (17) | 0.0132 (17) | 0.0229 (16) | 0.0069 (14) |
| C22 | 0.0327 (16) | 0.0310 (17) | 0.0212 (14) | 0.0097 (13) | −0.0035 (12) | −0.0036 (12) |
| C23 | 0.0491 (19) | 0.042 (2) | 0.0312 (16) | 0.0197 (15) | −0.0109 (14) | −0.0033 (14) |
| C24 | 0.0348 (17) | 0.0362 (18) | 0.0322 (16) | 0.0041 (14) | −0.0043 (13) | −0.0040 (13) |
| C25 | 0.0347 (16) | 0.0231 (15) | 0.0211 (13) | 0.0117 (12) | 0.0018 (12) | −0.0006 (11) |
| C26 | 0.077 (2) | 0.0380 (19) | 0.0302 (16) | 0.0336 (17) | −0.0023 (16) | −0.0064 (14) |
| C27 | 0.0388 (18) | 0.0384 (19) | 0.0464 (18) | 0.0213 (14) | −0.0010 (14) | 0.0007 (15) |

### Geometric parameters (Å, °)

| Bond/Distance | Value |
|---------------|-------|
| Br1—Si1       | 2.3185 (7) |
| Si1—Si2       | 2.4430 (10) |
| Si1—Si3       | 2.4448 (10) |
| Si1—Si4       | 2.4628 (9) |
| Si2—C4        | 1.908 (2) |
| Si2—C7        | 1.913 (3) |
| Si2—C1        | 1.914 (3) |
| Si3—C10       | 1.899 (3) |
| Si3—C13       | 1.899 (3) |
| Si3—C16       | 1.903 (3) |

| Bond/Distance | Value |
|---------------|-------|
| C12—H12B     | 0.9800 |
| C12—H12C     | 0.9800 |
| C13—C14      | 1.531 (4) |
| C13—C15      | 1.541 (4) |
| C13—H13      | 1.0000 |
| C14—H14A     | 0.9800 |
| C14—H14B     | 0.9800 |
| C14—H14C     | 0.9800 |
| C15—H15A     | 0.9800 |
| C15—H15B     | 0.9800 |
| Bond                  | Distance (Å) | Bond                  | Distance (Å) |
|----------------------|--------------|----------------------|--------------|
| Si4—C22              | 1.909 (3)    | C15—H15C             | 0.980        |
| Si4—C25              | 1.910 (3)    | C16—C17              | 1.533 (4)    |
| Si4—C19              | 1.911 (3)    | C16—C18              | 1.543 (4)    |
| C1—C2                | 1.532 (3)    | C16—H16              | 1.0000       |
| C1—C3                | 1.543 (4)    | C17—H17A             | 0.980        |
| C1—H1                | 1.0000       | C17—H17B             | 0.980        |
| C2—H2A               | 0.9800       | C17—H17C             | 0.980        |
| C2—H2B               | 0.9800       | C18—H18A             | 0.980        |
| C2—H2C               | 0.9800       | C18—H18B             | 0.980        |
| C3—H3A               | 0.9800       | C19—C20              | 1.530 (4)    |
| C3—H3B               | 0.9800       | C19—C21              | 1.539 (4)    |
| C4—C5                | 1.528 (4)    | C19—H19              | 1.0000       |
| C4—C6                | 1.536 (4)    | C20—H20A             | 0.980        |
| C4—H4                | 1.0000       | C20—H20B             | 0.980        |
| C5—H5A               | 0.9800       | C20—H20C             | 0.980        |
| C5—H5B               | 0.9800       | C21—H21A             | 0.980        |
| C5—H5C               | 0.9800       | C21—H21B             | 0.980        |
| C6—H6A               | 0.9800       | C21—H21C             | 0.980        |
| C6—H6B               | 0.9800       | C22—C23              | 1.525 (4)    |
| C6—H6C               | 0.9800       | C22—C24              | 1.538 (4)    |
| C7—C9                | 1.543 (4)    | C22—H22              | 1.0000       |
| C7—C8                | 1.544 (4)    | C23—H23A             | 0.980        |
| C7—H7                | 1.0000       | C23—H23B             | 0.980        |
| C8—H8A               | 0.9800       | C23—H23C             | 0.980        |
| C8—H8B               | 0.9800       | C24—H24A             | 0.980        |
| C8—H8C               | 0.9800       | C24—H24B             | 0.980        |
| C9—H9A               | 0.9800       | C24—H24C             | 0.980        |
| C9—H9B               | 0.9800       | C25—C27              | 1.525 (4)    |
| C9—H9C               | 0.9800       | C25—C26              | 1.543 (3)    |
| C10—C11              | 1.534 (4)    | C25—H25              | 1.0000       |
| C10—C12              | 1.541 (4)    | C26—H26A             | 0.980        |
| C10—H10              | 1.0000       | C26—H26B             | 0.980        |
| C11—H11A             | 0.9800       | C26—H26C             | 0.980        |
| C11—H11B             | 0.9800       | C27—H27A             | 0.980        |
| C11—H11C             | 0.9800       | C27—H27B             | 0.980        |
| C12—H12A             | 0.9800       | C27—H27C             | 0.980        |
| Br1—Si1—Si2          | 103.77 (3)   | C10—C12—H12C         | 109.5        |
| Br1—Si1—Si3          | 98.44 (3)    | H12A—C12—H12C        | 109.5        |
| Si2—Si1—Si3          | 116.55 (3)   | H12B—C12—H12C        | 109.5        |
| Br1—Si1—Si4          | 102.65 (3)   | C14—C13—C15          | 109.5 (2)    |
| Si2—Si1—Si4          | 115.02 (4)   | C14—C13—Si3          | 112.65 (19)  |
| Si3—Si1—Si4          | 116.59 (4)   | C15—C13—Si3          | 116.31 (18)  |
| C4—Si2—C7            | 108.70 (11)  | C14—C13—H13          | 105.9        |
| C4—Si2—C1            | 111.49 (12)  | C15—C13—H13          | 105.9        |
| C7—Si2—C1            | 109.69 (11)  | Si3—C13—H13          | 105.9        |
| C4—Si2—Si1           | 112.06 (9)   | C13—C14—H14A         | 109.5        |
| Bond                  | Angle (deg) | Bond                  | Angle (deg) |
|----------------------|------------|----------------------|------------|
| C7—Si2—Si1           | 106.40 (9) | C13—C14—H14B         | 109.5      |
| C1—Si2—Si1           | 108.35 (8) | H14A—C14—H14B        | 109.5      |
| C10—Si3—C13          | 111.22 (12)| C13—C14—H14C         | 109.5      |
| C10—Si3—C16          | 109.44 (12)| H14A—C14—H14C        | 109.5      |
| C13—Si3—C16          | 111.50 (12)| H14B—C14—H14C        | 109.5      |
| C10—Si3—Si1          | 107.75 (9) | C13—C15—H15A         | 109.5      |
| C13—Si3—Si1          | 109.78 (8) | C13—C15—H15B         | 109.5      |
| C16—Si3—Si1          | 106.98 (9) | H15A—C15—H15B        | 109.5      |
| C22—Si4—C25          | 104.78 (12)| C13—C15—H15C         | 109.5      |
| C22—Si4—C19          | 106.42 (12)| H15A—C15—H15C        | 109.5      |
| C25—Si4—C19          | 111.59 (12)| H15B—C15—H15C        | 109.5      |
| C22—Si4—Si1          | 112.92 (8) | C17—C16—C18          | 108.9 (2)  |
| C25—Si4—Si1          | 111.74 (8) | C17—C16—Si3          | 116.29 (19)|
| C19—Si4—Si1          | 109.24 (8) | C18—C16—Si3          | 112.56 (18)|
| C2—C1—C3             | 107.7 (2)  | C17—C16—H16          | 106.1      |
| C2—C1—Si2            | 115.52 (18)| C18—C16—H16          | 106.1      |
| C3—C1—Si2            | 114.54 (18)| Si3—C16—H16          | 106.1      |
| C2—C1—H1             | 106.1      | C16—C17—H17A         | 109.5      |
| C3—C1—H1             | 106.1      | C16—C17—H17B         | 109.5      |
| Si2—C1—H1            | 106.1      | H17A—C17—H17B        | 109.5      |
| C1—C2—H2A            | 109.5      | C16—C17—H17C         | 109.5      |
| C1—C2—H2B            | 109.5      | H17A—C17—H17C        | 109.5      |
| H2A—C2—H2B           | 109.5      | H17B—C17—H17C        | 109.5      |
| C1—C2—H2C            | 109.5      | C16—C18—H18A         | 109.5      |
| H2A—C2—H2C           | 109.5      | C16—C18—H18B         | 109.5      |
| H2B—C2—H2C           | 109.5      | H18A—C18—H18B        | 109.5      |
| C1—C3—H3A            | 109.5      | C16—C18—H18C         | 109.5      |
| C1—C3—H3B            | 109.5      | H18A—C18—H18C        | 109.5      |
| H3A—C3—H3B           | 109.5      | H18B—C18—H18C        | 109.5      |
| C1—C3—H3C            | 109.5      | C20—C19—C21          | 109.0 (2)  |
| H3A—C3—H3C           | 109.5      | C20—C19—Si4          | 113.92 (19)|
| H3B—C3—H3C           | 109.5      | C21—C19—Si4          | 114.62 (19)|
| C5—C4—C6             | 108.5 (2)  | C20—C19—H19          | 106.2      |
| C5—C4—Si2            | 114.13 (17)| C21—C19—H19          | 106.2      |
| C6—C4—Si2            | 114.24 (19)| Si4—C19—H19          | 106.2      |
| C5—C4—H4             | 106.5      | C19—C20—H20A         | 109.5      |
| C6—C4—H4             | 106.5      | C19—C20—H20B         | 109.5      |
| Si2—C4—H4            | 106.5      | H20A—C20—H20B        | 109.5      |
| C4—C5—H5A            | 109.5      | C19—C20—H20C         | 109.5      |
| C4—C5—H5B            | 109.5      | H20A—C20—H20C        | 109.5      |
| H5A—C5—H5B           | 109.5      | H20B—C20—H20C        | 109.5      |
| C4—C5—H5C            | 109.5      | C19—C21—H21A         | 109.5      |
| H5A—C5—H5C           | 109.5      | C19—C21—H21B         | 109.5      |
| H5B—C5—H5C           | 109.5      | H21A—C21—H21B        | 109.5      |
| C4—C6—H6A            | 109.5      | C19—C21—H21C         | 109.5      |
| C4—C6—H6B            | 109.5      | H21A—C21—H21C        | 109.5      |
| H6A—C6—H6B           | 109.5      | H21B—C21—H21C        | 109.5      |
| C4—C6—H6C            | 109.5      | C23—C22—C24          | 110.6 (2)  |
H6A—C6—H6C 109.5  C23—C22—Si4 116.47 (19)
H6B—C6—H6C 109.5  C24—C22—Si4 115.61 (18)
C9—C7—C8 109.7 (2)  C23—C22—H22 104.1
C9—C7—Si2 115.43 (18)  C24—C22—H22 104.1
C8—C7—Si2 114.49 (19)  Si4—C22—H22 104.1
C9—C7—H7 105.4  C22—C23—H23A 109.5
C8—C7—H7 105.4  C22—C23—H23B 109.5
Si2—C7—H7 105.4  C23—C23—H23B 109.5
C7—C8—H8A 109.5  C22—C23—H23C 109.5
C7—C8—H8B 109.5  H23A—C23—H23B 109.5
H8A—C8—H8B 109.5  H23A—C23—H23C 109.5
C7—C8—H8C 109.5  C22—C24—H24A 109.5
H8A—C8—H8C 109.5  C22—C24—H24B 109.5
H8B—C8—H8C 109.5  C22—C24—H24C 109.5
C9—C7—H7 109.5  C23—C22—Si4 116.47 (19)
C9—C7—H7 109.5  C23—C22—H22 104.1
Si2—C7—H7 109.5  C24—C22—Si4 115.61 (18)
C7—C8—H8A 109.5  C24—C22—H22 104.1
C7—C8—H8B 109.5  H24A—C24—H24B 109.5
H8A—C8—H8B 109.5  H24A—C24—H24C 109.5
C7—C8—H8C 109.5  C24—C24—H24C 109.5
H8A—C8—H8C 109.5  C24—C24—H24B 109.5
H8B—C8—H8C 109.5  C24—C24—H24A 109.5
C9—C7—H7 109.5  C25—C22—Si4 116.47 (19)
C9—C7—H7 109.5  C25—C22—H22 104.1
Si2—C7—H7 109.5  C26—C22—Si4 115.61 (18)
C7—C8—H8A 109.5  C26—C22—H22 104.1
C7—C8—H8B 109.5  H26A—C26—H26B 109.5
H8A—C8—H8B 109.5  H26A—C26—H26C 109.5
C7—C8—H8C 109.5  C26—C26—H26B 109.5
H8A—C8—H8C 109.5  C26—C26—H26C 109.5
H8B—C8—H8C 109.5  C26—C26—H26A 109.5
C11—C10—C12 110.3 (2)  C27—C25—Si4 117.05 (18)
C11—C10—Si3 112.34 (19)  C27—C25—H25 106.0
C12—C10—Si3 115.08 (19)  Si4—C25—H25 106.0
C11—C10—H10 106.1  C25—C25—H25 106.0
C12—C10—H10 106.1  C26—C25—H25 106.0
Si3—C10—H10 106.1  Si4—C25—H25 106.0
C10—C11—H11A 109.5  C25—C26—H26A 109.5
C10—C11—H11B 109.5  C25—C26—H26B 109.5
H11A—C11—H11B 109.5  C25—C26—H26C 109.5
H11A—C11—H11B 109.5  H26B—C26—H26A 109.5
C10—C11—H11C 109.5  H26B—C26—H26C 109.5
H11B—C11—H11C 109.5  C25—C27—H27A 109.5
C10—C12—H12A 109.5  C25—C27—H27B 109.5
C10—C12—H12B 109.5  C25—C27—H27C 109.5
H12A—C12—H12B 109.5  H27A—C27—H27B 109.5
H12A—C12—H12B 109.5  H27B—C27—H27C 109.5
C13—Si3—C10—C11 −172.26 (19)  C10—Si3—C13—C14 −52.9 (2)
C16—Si3—C10—C11 −48.6 (2)  C16—Si3—C13—C14 −175.32 (19)
Si1—Si3—C10—C11 67.4 (2)  Si1—Si3—C13—C14 66.3 (2)
C13—Si3—C10—C12 −44.9 (2)  C10—Si3—C13—C15 74.7 (2)
C16—Si3—C10—C12 78.8 (2)  C16—Si3—C13—C15 −47.8 (2)
Si1—Si3—C10—C12 −165.25 (18)  Si1—Si3—C13—C15 −166.17 (17)

Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|--------|
| C5—H5B···Br1 | 0.98 | 2.80  | 3.711 (3) | 155 |
| C16—H16···Br1 | 1.00 | 2.84  | 3.584 (3) | 131 |
|          |        |      |      |      |
|----------|--------|------|------|------|
| C23—H23A⋯Br1 | 0.98   | 2.87 | 3.685 (3) | 142  |
| C24—H24C⋯Br1  | 0.98   | 2.93 | 3.726 (3) | 139  |