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# Crystal structure of 1,1,2,2-tetramethyl-1,2-bis(2,3,4,5-tetramethylcyclopenta-2,4-dien-1-yl)disilane

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The molecular structure of the title compound,  $C_{22}H_{38}Si_2$ , features a *trans* arrangement of the cyclopentadienyl rings to avoid steric strain [C-Si-Si-C torsion angle = -179.0 (5)°]. The Si-Si bond length is 2.3444 (4) Å. The most notable intermolecular interactions in the molecular packing are C- $H\cdots\pi$  contacts that lead to the formation of wave-like supramolecular chains along the *b* axis.

Keywords: crystal structure; disilane; ansa ligand.

CCDC reference: 1432476

#### 1. Related literature

For synthesis of the title compound, see: Kessler *et al.* (2013). For group 4 complexes with this ligand, see: Godemann *et al.* (2014, 2015); Pinkas *et al.* (2011); Xu *et al.* (1997); Horáček *et al.* (2008).

#### 2. Experimental

#### 2.1. Crystal data

 $C_{22}H_{38}Si_2$  $M_r = 358.70$  Monoclinic  $P2_1/n$ a = 8.7790 (2) Å b = 15.3039 (4) Å c = 16.4355 (4) Å  $\beta = 93.678 \text{ (1)}^{\circ}$   $V = 2203.61 \text{ (9) Å}^{3}$ Z = 4 Mo  $K\alpha$  radiation  $\mu = 0.16 \text{ mm}^{-1}$  T = 150 K $0.55 \times 0.41 \times 0.29 \text{ mm}$ 

#### 2.2. Data collection

Bruker APEXII CCD diffractometer Absorption correction: multi-scan (SADABS; Bruker, 2008)  $T_{\min} = 0.92$ ,  $T_{\max} = 0.95$ 

46817 measured reflections 5318 independent reflections 4636 reflections with  $I > 2\sigma(I)$   $R_{\rm int} = 0.035$ 

#### 2.3. Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.034$   $wR(F^2) = 0.097$  S = 1.065318 reflections

229 parameters H-atom parameters constrained  $\Delta \rho_{\rm max} = 0.32 \ {\rm e \ \mathring{A}^{-3}}$ 

 $\Delta \rho_{\text{max}} = 0.32 \text{ e Å}^{-3}$  $\Delta \rho_{\text{min}} = -0.23 \text{ e Å}^{-3}$ 

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

Cg1 is the centroid of the C14-C18 ring.

| $D$ $ H$ $\cdots$ $A$ | D-H  | $H \cdot \cdot \cdot A$ | $D \cdot \cdot \cdot A$ | $D-\mathrm{H}\cdots A$ |
|-----------------------|------|-------------------------|-------------------------|------------------------|
| $C1-H1\cdots Cg1^{i}$ | 1.00 | 2.76                    | 3.7350 (13)             | 166                    |

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

Data collection: *APEX2* (Bruker, 2011); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

#### Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: TK5400).

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## Crystal structure of 1,1,2,2-tetramethyl-1,2-bis(2,3,4,5-tetramethylcyclopenta-2,4-dien-1-yl)disilane

#### **Christian Godemann, Anke Spannenberg and Torsten Beweries**

#### S1. Synthesis and crystallization

The synthesis of the title compound has been described previously (Kessler *et al.*, 2013). A saturated solution of the title compound in n-hexane was very slowly cooled from 60 °C to room temperature resulting in precipitation of colourless crystals.

#### S2. Refinement

H atoms were placed in idealized positions with  $d(C—H) = 1.00 \text{ Å (CH)} \& 0.98 \text{ Å (CH}_3)$ , and refined using a riding model with  $U_{iso}(H)$  fixed at 1.2  $U_{eq}(C)$  for CH & 1.5  $U_{eq}(C)$  for CH<sub>3</sub>.

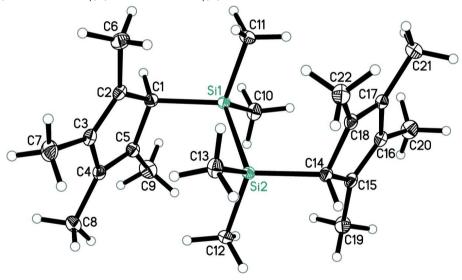


Figure 1

Molecular structure of the title compound with atom labelling scheme and displacement ellipsoids drawn at 30% probability level.

1,1,2,2-Tetramethyl-1,2-bis(2,3,4,5-tetramethylcyclopenta-2,4-dien-1-yl)disilane

#### Crystal data

 $C_{22}H_{38}Si_2$  c = 16.4355 (4) Å  $M_r = 358.70$   $\beta = 93.678 (1)^{\circ}$  Monoclinic,  $P2_1/n$   $V = 2203.61 (9) Å^3$  a = 8.7790 (2) Å Z = 4 b = 15.3039 (4) Å F(000) = 792

 $D_x$  = 1.081 Mg m<sup>-3</sup> Mo  $K\alpha$  radiation,  $\lambda$  = 0.71073 Å Cell parameters from 9858 reflections  $\theta$  = 2.5–28.6°  $\mu = 0.16 \text{ mm}^{-1}$  T = 150 KPrism, colourless  $0.55 \times 0.41 \times 0.29 \text{ mm}$ 

Data collection

Bruker APEXII CCD diffractometer Radiation source: fine-focus sealed tube Curved graphite monochromator Detector resolution: 8.3333 pixels mm $^{-1}$   $\varphi$  and  $\omega$  scans

 $\varphi$  and  $\omega$  scans
Absorption correction: multi-scan
(SADABS; Bruker, 2008)  $T_{\min} = 0.92, T_{\max} = 0.95$ 

46817 measured reflections 5318 independent reflections 4636 reflections with  $I > 2\sigma(I)$   $R_{\text{int}} = 0.035$   $\theta_{\text{max}} = 28.0^{\circ}, \theta_{\text{min}} = 1.8^{\circ}$   $h = -11 \rightarrow 11$   $k = -20 \rightarrow 19$  $l = -21 \rightarrow 21$ 

Refinement

Refinement on  $F^2$ Least-squares matrix: full  $R[F^2 > 2\sigma(F^2)] = 0.034$   $wR(F^2) = 0.097$  S = 1.065318 reflections 229 parameters 0 restraints Primary atom site location: structure-invariant

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained  $w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 0.8183P]$ where  $P = (F_o^2 + 2F_c^2)/3$   $(\Delta/\sigma)_{\text{max}} = 0.001$   $\Delta\rho_{\text{max}} = 0.32 \text{ e Å}^{-3}$   $\Delta\rho_{\text{min}} = -0.23 \text{ e Å}^{-3}$ 

Secondary atom site location: difference Fourier

Special details

direct methods

**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  $F^2 > \sigma(F^2)$  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 F-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters  $(\hat{A}^2)$ 

|     | x            | У            | Z            | $U_{ m iso}$ */ $U_{ m eq}$ |
|-----|--------------|--------------|--------------|-----------------------------|
| C1  | 0.85658 (13) | 0.71127 (8)  | 0.10459 (7)  | 0.0212 (2)                  |
| H1  | 0.8437       | 0.6501       | 0.1244       | 0.025*                      |
| C2  | 1.01814 (13) | 0.72631 (8)  | 0.08367 (8)  | 0.0227 (2)                  |
| C3  | 1.01837 (14) | 0.75224 (8)  | 0.00516 (8)  | 0.0243 (2)                  |
| C4  | 0.86221 (14) | 0.75132 (8)  | -0.03149(7)  | 0.0234 (2)                  |
| C5  | 0.76715 (14) | 0.72439 (8)  | 0.02488 (7)  | 0.0228 (2)                  |
| C6  | 1.15522 (16) | 0.71322 (10) | 0.14202 (9)  | 0.0349 (3)                  |
| H6A | 1.2403       | 0.6908       | 0.1123       | 0.052*                      |
| H6B | 1.1304       | 0.6712       | 0.1842       | 0.052*                      |
| Н6С | 1.1843       | 0.7691       | 0.1676       | 0.052*                      |
| C7  | 1.15333 (17) | 0.77834 (11) | -0.04066(10) | 0.0374 (3)                  |
| H7A | 1.2463       | 0.7744       | -0.0045      | 0.056*                      |

| Н7В   | 1.1400       | 0.8385       | -0.0601      | 0.056*     |
|-------|--------------|--------------|--------------|------------|
| H7C   | 1.1620       | 0.7392       | -0.0873      | 0.056*     |
| C8    | 0.81945 (17) | 0.77582 (10) | -0.11828 (8) | 0.0332 (3) |
| H8A   | 0.8533       | 0.7299       | -0.1546      | 0.050*     |
| H8B   | 0.8687       | 0.8312       | -0.1311      | 0.050*     |
| H8C   | 0.7084       | 0.7823       | -0.1259      | 0.050*     |
| C9    | 0.59858 (16) | 0.70960 (11) | 0.01139 (9)  | 0.0359 (3) |
| H9A   | 0.5448       | 0.7653       | 0.0159       | 0.054*     |
| H9B   | 0.5648       | 0.6688       | 0.0525       | 0.054*     |
| H9C   | 0.5760       | 0.6850       | -0.0431      | 0.054*     |
| C10   | 0.59182 (15) | 0.77168 (9)  | 0.20801 (9)  | 0.0298 (3) |
| H10A  | 0.5796       | 0.7097       | 0.2212       | 0.045*     |
| H10B  | 0.5237       | 0.7867       | 0.1605       | 0.045*     |
| H10C  | 0.5661       | 0.8075       | 0.2546       | 0.045*     |
| C11   | 0.91263 (16) | 0.77522 (9)  | 0.28252 (8)  | 0.0283 (3) |
| H11A  | 0.8710       | 0.8103       | 0.3258       | 0.042*     |
| H11B  | 1.0184       | 0.7928       | 0.2756       | 0.042*     |
| H11C  | 0.9099       | 0.7132       | 0.2973       | 0.042*     |
| C12   | 0.69980 (16) | 0.95635 (9)  | 0.04136 (7)  | 0.0275 (3) |
| H12A  | 0.6950       | 1.0192       | 0.0299       | 0.041*     |
| H12B  | 0.5966       | 0.9340       | 0.0475       | 0.041*     |
| H12C  | 0.7448       | 0.9260       | -0.0038      | 0.041*     |
| C13   | 1.02293 (15) | 0.96094 (9)  | 0.11437 (8)  | 0.0281 (3) |
| H13A  | 1.0465       | 0.9302       | 0.0644       | 0.042*     |
| H13B  | 1.0925       | 0.9412       | 0.1597       | 0.042*     |
| H13C  | 1.0353       | 1.0240       | 0.1066       | 0.042*     |
| C14   | 0.76149 (13) | 1.01788 (8)  | 0.21979 (7)  | 0.0205 (2) |
| H14   | 0.7769       | 1.0788       | 0.1999       | 0.025*     |
| C15   | 0.59856 (13) | 1.00765 (8)  | 0.24095 (7)  | 0.0223 (2) |
| C16   | 0.59561 (14) | 0.98747 (8)  | 0.32073 (8)  | 0.0236 (2) |
| C17   | 0.75209 (14) | 0.98656 (8)  | 0.35759 (7)  | 0.0228 (2) |
| C18   | 0.84985 (13) | 1.00645 (8)  | 0.30048 (7)  | 0.0222 (2) |
| C19   | 0.46292 (15) | 1.01960 (10) | 0.18157 (9)  | 0.0334 (3) |
| H19A  | 0.4372       | 0.9637       | 0.1550       | 0.050*     |
| H19B  | 0.4872       | 1.0627       | 0.1403       | 0.050*     |
| H19C  | 0.3758       | 1.0402       | 0.2107       | 0.050*     |
| C20   | 0.45939 (16) | 0.97111 (10) | 0.36880 (10) | 0.0367 (3) |
| H20A  | 0.4494       | 1.0185       | 0.4082       | 0.055*     |
| H20B  | 0.4722       | 0.9155       | 0.3979       | 0.055*     |
| H20C  | 0.3674       | 0.9686       | 0.3318       | 0.055*     |
| C21   | 0.78832 (18) | 0.96916 (10) | 0.44647 (8)  | 0.0346 (3) |
| H21A  | 0.8990       | 0.9635       | 0.4570       | 0.052*     |
| H21B  | 0.7385       | 0.9149       | 0.4620       | 0.052*     |
| H21C  | 0.7511       | 1.0177       | 0.4786       | 0.052*     |
| C22   | 1.01980 (15) | 1.01596 (10) | 0.31332 (9)  | 0.0324 (3) |
| H22A  | 1.0463       | 1.0338       | 0.3697       | 0.0324 (3) |
| H22B  | 1.0554       | 1.0604       | 0.2760       | 0.049*     |
| H22C  | 1.0687       | 0.9599       | 0.3026       | 0.049*     |
| 11220 | 1.000/       | 0.9399       | 0.3020       | U.UT2      |

| Si1 | 0.79503 (4) | 0.79312 (2) | 0.184414 (19) | 0.01845 (9) |
|-----|-------------|-------------|---------------|-------------|
| Si2 | 0.82065 (4) | 0.93696 (2) | 0.138159 (18) | 0.01799 (9) |

#### Atomic displacement parameters $(\mathring{A}^2)$

|     | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$      | $U^{13}$     | $U^{23}$     |
|-----|--------------|--------------|--------------|---------------|--------------|--------------|
| C1  | 0.0224 (6)   | 0.0182 (5)   | 0.0231 (6)   | -0.0005 (4)   | 0.0010(4)    | 0.0000 (4)   |
| C2  | 0.0193 (6)   | 0.0207 (5)   | 0.0281 (6)   | 0.0035 (4)    | 0.0009 (5)   | -0.0026(5)   |
| C3  | 0.0220(6)    | 0.0228 (6)   | 0.0287 (6)   | 0.0019 (4)    | 0.0058 (5)   | -0.0031(5)   |
| C4  | 0.0253 (6)   | 0.0226 (6)   | 0.0223 (6)   | 0.0024 (5)    | 0.0009 (5)   | -0.0038(5)   |
| C5  | 0.0219 (6)   | 0.0223 (6)   | 0.0239 (6)   | -0.0014(4)    | -0.0015(4)   | -0.0046(5)   |
| C6  | 0.0237 (6)   | 0.0428 (8)   | 0.0373 (7)   | 0.0086 (6)    | -0.0046(5)   | -0.0002(6)   |
| C7  | 0.0292 (7)   | 0.0442 (8)   | 0.0402 (8)   | 0.0019 (6)    | 0.0139 (6)   | 0.0004(6)    |
| C8  | 0.0373 (7)   | 0.0390(8)    | 0.0231 (6)   | 0.0037 (6)    | 0.0014 (5)   | -0.0008(5)   |
| C9  | 0.0250 (7)   | 0.0465 (8)   | 0.0354 (7)   | -0.0099(6)    | -0.0042(5)   | -0.0049(6)   |
| C10 | 0.0259 (6)   | 0.0287 (7)   | 0.0359 (7)   | -0.0050(5)    | 0.0114 (5)   | -0.0005(5)   |
| C11 | 0.0353 (7)   | 0.0288 (6)   | 0.0204(6)    | 0.0030(5)     | -0.0022(5)   | 0.0033 (5)   |
| C12 | 0.0346 (7)   | 0.0277 (6)   | 0.0200(6)    | 0.0040 (5)    | -0.0011(5)   | 0.0023 (5)   |
| C13 | 0.0264 (6)   | 0.0264 (6)   | 0.0328 (7)   | -0.0051(5)    | 0.0113 (5)   | -0.0022(5)   |
| C14 | 0.0195 (5)   | 0.0203 (5)   | 0.0215 (5)   | 0.0016 (4)    | 0.0004 (4)   | -0.0023(4)   |
| C15 | 0.0176 (5)   | 0.0216 (6)   | 0.0273 (6)   | 0.0035 (4)    | -0.0006(4)   | -0.0049(5)   |
| C16 | 0.0217 (6)   | 0.0203 (5)   | 0.0290(6)    | 0.0012 (4)    | 0.0040 (5)   | -0.0033(5)   |
| C17 | 0.0260(6)    | 0.0199 (5)   | 0.0222 (6)   | 0.0033 (4)    | -0.0003(5)   | -0.0028(4)   |
| C18 | 0.0201 (6)   | 0.0215 (5)   | 0.0244 (6)   | 0.0021 (4)    | -0.0024(4)   | -0.0060(5)   |
| C19 | 0.0222 (6)   | 0.0429 (8)   | 0.0342 (7)   | 0.0080(6)     | -0.0059(5)   | -0.0073 (6)  |
| C20 | 0.0292 (7)   | 0.0395 (8)   | 0.0427 (8)   | -0.0005 (6)   | 0.0126 (6)   | 0.0018 (6)   |
| C21 | 0.0422 (8)   | 0.0362 (7)   | 0.0249 (6)   | 0.0042 (6)    | -0.0009(6)   | 0.0012 (6)   |
| C22 | 0.0205 (6)   | 0.0409 (8)   | 0.0351 (7)   | 0.0000 (5)    | -0.0042(5)   | -0.0099(6)   |
| Si1 | 0.01894 (16) | 0.01846 (16) | 0.01803 (16) | -0.00115 (11) | 0.00177 (11) | 0.00206 (11) |
| Si2 | 0.01903 (16) | 0.01773 (16) | 0.01736 (15) | -0.00037(11)  | 0.00222 (11) | 0.00092 (11) |

#### Geometric parameters (Å, °)

| C1—C5  | 1.4969 (16) | C12—H12A | 0.9800      |
|--------|-------------|----------|-------------|
| C1—C2  | 1.4985 (16) | C12—H12B | 0.9800      |
| C1—Si1 | 1.9166 (12) | C12—H12C | 0.9800      |
| C1—H1  | 1.0000      | C13—Si2  | 1.8789 (13) |
| C2—C3  | 1.3501 (18) | C13—H13A | 0.9800      |
| C2—C6  | 1.5033 (17) | C13—H13B | 0.9800      |
| C3—C4  | 1.4617 (17) | C13—H13C | 0.9800      |
| C3—C7  | 1.4984 (18) | C14—C15  | 1.5017 (16) |
| C4—C5  | 1.3505 (17) | C14—C18  | 1.5031 (16) |
| C4—C8  | 1.4993 (17) | C14—Si2  | 1.9216 (12) |
| C5—C9  | 1.4994 (17) | C14—H14  | 1.0000      |
| C6—H6A | 0.9800      | C15—C16  | 1.3490 (17) |
| C6—H6B | 0.9800      | C15—C19  | 1.5016 (17) |
| C6—H6C | 0.9800      | C16—C17  | 1.4655 (17) |
| C7—H7A | 0.9800      | C16—C20  | 1.4961 (17) |
|        |             |          |             |

| C7—H7B     | 0.9800      | C17—C18                    | 1.3467 (17) |
|------------|-------------|----------------------------|-------------|
| C7—H7C     | 0.9800      | C17—C21                    | 1.4989 (17) |
| C8—H8A     | 0.9800      | C18—C22                    | 1.5004 (17) |
| C8—H8B     | 0.9800      | C19—H19A                   | 0.9800      |
| C8—H8C     | 0.9800      | C19—H19B                   | 0.9800      |
| C9—H9A     | 0.9800      | C19—H19C                   | 0.9800      |
| C9—H9B     | 0.9800      | C20—H20A                   | 0.9800      |
| С9—Н9С     | 0.9800      | C20—H20B                   | 0.9800      |
| C10—Si1    | 1.8787 (13) | C20—H20C                   | 0.9800      |
| C10—H10A   | 0.9800      | C21—H21A                   | 0.9800      |
| C10—H10B   | 0.9800      | C21—H21B                   | 0.9800      |
| C10—H10C   | 0.9800      | C21—H21C                   | 0.9800      |
|            |             |                            |             |
| C11—Si1    | 1.8780 (13) | C22—H22A                   | 0.9800      |
| C11—H11A   | 0.9800      | C22—H22B                   | 0.9800      |
| C11—H11B   | 0.9800      | C22—H22C                   | 0.9800      |
| C11—H11C   | 0.9800      | Si1—Si2                    | 2.3444 (4)  |
| C12—Si2    | 1.8783 (13) |                            |             |
| C5 C1 C2   | 102.20 (10) | S:2 C12 H12A               | 100.5       |
| C5—C1—C2   | 103.28 (10) | Si2—C13—H13A               | 109.5       |
| C5—C1—Si1  | 110.87 (8)  | Si2—C13—H13B               | 109.5       |
| C2—C1—Si1  | 111.67 (8)  | H13A—C13—H13B              | 109.5       |
| C5—C1—H1   | 110.3       | Si2—C13—H13C               | 109.5       |
| C2—C1—H1   | 110.3       | H13A—C13—H13C              | 109.5       |
| Si1—C1—H1  | 110.3       | H13B—C13—H13C              | 109.5       |
| C3—C2—C1   | 108.89 (11) | C15—C14—C18                | 103.23 (10) |
| C3—C2—C6   | 126.77 (12) | C15—C14—Si2                | 113.49 (8)  |
| C1—C2—C6   | 124.33 (11) | C18—C14—Si2                | 113.19 (8)  |
| C2—C3—C4   | 109.40 (11) | C15—C14—H14                | 108.9       |
| C2—C3—C7   | 127.48 (12) | C18—C14—H14                | 108.9       |
| C4—C3—C7   | 123.12 (12) | Si2—C14—H14                | 108.9       |
| C5—C4—C3   | 108.95 (11) | C16—C15—C19                | 126.57 (12) |
| C5—C4—C8   | 126.95 (12) | C16—C15—C14                | 109.08 (10) |
| C3—C4—C8   | 124.10 (12) | C19—C15—C14                | 124.35 (11) |
| C4—C5—C1   | 109.19 (11) | C15—C16—C17                | 109.15 (11) |
| C4—C5—C9   | 126.30 (12) | C15—C16—C20                | 128.13 (12) |
| C1—C5—C9   | 124.51 (11) | C17—C16—C20                | 122.68 (12) |
| C2—C6—H6A  | 109.5       | C18—C17—C16                | 109.40 (11) |
| C2—C6—H6B  | 109.5       | C18—C17—C21                | 127.92 (12) |
| H6A—C6—H6B | 109.5       | C16—C17—C21                | 122.63 (11) |
| C2—C6—H6C  | 109.5       | C17—C18—C22                | 126.61 (12) |
| H6A—C6—H6C | 109.5       | C17—C18—C22<br>C17—C18—C14 | * *         |
|            |             |                            | 108.99 (10) |
| H6B—C6—H6C | 109.5       | C22—C18—C14                | 124.40 (11) |
| C3—C7—H7A  | 109.5       | C15—C19—H19A               | 109.5       |
| C3—C7—H7B  | 109.5       | C15—C19—H19B               | 109.5       |
| H7A—C7—H7B | 109.5       | H19A—C19—H19B              | 109.5       |
| C3—C7—H7C  | 109.5       | C15—C19—H19C               | 109.5       |
| H7A—C7—H7C | 109.5       | H19A—C19—H19C              | 109.5       |
| H7B—C7—H7C | 109.5       | H19B—C19—H19C              | 109.5       |
|            |             |                            |             |

| C4—C8—H8A                            | 109.5        | C16—C20—H20A              | 109.5        |
|--------------------------------------|--------------|---------------------------|--------------|
| C4—C8—H8B                            | 109.5        | C16—C20—H20B              | 109.5        |
| H8A—C8—H8B                           | 109.5        | H20A—C20—H20B             | 109.5        |
| C4—C8—H8C                            | 109.5        | C16—C20—H20C              | 109.5        |
| H8A—C8—H8C                           | 109.5        | H20A—C20—H20C             | 109.5        |
| H8B—C8—H8C                           | 109.5        | H20B—C20—H20C             | 109.5        |
| C5—C9—H9A                            | 109.5        | C17—C21—H21A              | 109.5        |
| C5—C9—H9B                            | 109.5        | C17—C21—H21B              | 109.5        |
| H9A—C9—H9B                           | 109.5        | H21A—C21—H21B             | 109.5        |
| C5—C9—H9C                            | 109.5        | C17—C21—H21C              | 109.5        |
| H9A—C9—H9C                           | 109.5        | H21A—C21—H21C             | 109.5        |
| H9B—C9—H9C                           | 109.5        | H21B—C21—H21C             | 109.5        |
| Si1—C10—H10A                         | 109.5        | C18—C22—H22A              | 109.5        |
| Si1—C10—H10B                         | 109.5        | C18—C22—H22B              | 109.5        |
| H10A—C10—H10B                        | 109.5        | H22A—C22—H22B             | 109.5        |
| Si1—C10—H10C                         | 109.5        | C18—C22—H22C              | 109.5        |
| H10A—C10—H10C                        | 109.5        | H22A—C22—H22C             | 109.5        |
| H10B—C10—H10C                        | 109.5        | H22B—C22—H22C             | 109.5        |
| Si1—C11—H11A                         | 109.5        | C11—Si1—C10               | 109.3        |
| Si1—C11—H11B                         |              | C11—Si1—C10 C11—Si1—C1    | ` '          |
|                                      | 109.5        |                           | 109.20 (6)   |
| H11A—C11—H11B                        | 109.5        | C10—Si1—C1<br>C11—Si1—Si2 | 109.90 (6)   |
| Si1—C11—H11C                         | 109.5        |                           | 110.88 (4)   |
| H11A—C11—H11C                        | 109.5        | C10—Si1—Si2               | 110.06 (5)   |
| H11B—C11—H11C                        | 109.5        | C1—Si1—Si2                | 110.77 (4)   |
| Si2—C12—H12A                         | 109.5        | C12—Si2—C13               | 106.44 (6)   |
| Si2—C12—H12B                         | 109.5        | C12—Si2—C14               | 109.04 (6)   |
| H12A—C12—H12B                        | 109.5        | C13—Si2—C14               | 108.71 (6)   |
| Si2—C12—H12C                         | 109.5        | C12—Si2—Si1               | 111.24 (4)   |
| H12A—C12—H12C                        | 109.5        | C13—Si2—Si1               | 111.25 (4)   |
| H12B—C12—H12C                        | 109.5        | C14—Si2—Si1               | 110.05 (4)   |
| C5—C1—C2—C3                          | 4.99 (13)    | C20—C16—C17—C21           | -0.01 (19)   |
| Si1—C1—C2—C3                         | -114.20 (10) | C16—C17—C18—C22           | 177.49 (12)  |
| C5—C1—C2—C6                          | -174.52 (12) | C21—C17—C18—C22           | -0.1(2)      |
| Si1—C1—C2—C6                         | 66.29 (14)   | C16—C17—C18—C14           | -2.63(14)    |
| C1—C2—C3—C4                          | -3.13 (14)   | C21—C17—C18—C14           | 179.77 (12)  |
| C6—C2—C3—C4                          | 176.37 (12)  | C15—C14—C18—C17           | 3.78 (13)    |
| C1—C2—C3—C7                          | 177.06 (12)  | Si2—C14—C18—C17           | -119.32 (10) |
| C6—C2—C3—C7                          | -3.4(2)      | C15—C14—C18—C22           | -176.33 (11) |
| C2—C3—C4—C5                          | -0.26 (15)   | Si2—C14—C18—C22           | 60.57 (14)   |
| C7—C3—C4—C5                          | 179.56 (12)  | C5—C1—Si1—C11             | -179.05 (8)  |
| C2—C3—C4—C8                          | -179.61 (12) | C2—C1—Si1—C11             | -64.46 (10)  |
| C7—C3—C4—C8                          | 0.2 (2)      | C5—C1—Si1—C10             | 65.17 (10)   |
| C3—C4—C5—C1                          | 3.55 (14)    | C2—C1—Si1—C10             | 179.76 (9)   |
| C8—C4—C5—C1                          | -177.13 (12) | C5—C1—Si1—Si2             | -56.66 (9)   |
| C3—C4—C5—C9                          | -176.51 (12) | C2—C1—Si1—Si2             | 57.93 (9)    |
| C8—C4—C5—C9                          | 2.8 (2)      | C15—C14—Si2—C12           | 61.62 (10)   |
| C2—C1—C5—C4                          | -5.18 (13)   | C18—C14—Si2—C12           | 178.86 (9)   |
| 02-01-03 <del>-</del> 0 <del>1</del> | 5.10 (15)    | C10 C1 <del>1</del> -512  | 1 / 0.00 (3) |

| Si1—C1—C5—C4    | 114.56 (10)  | C15—C14—Si2—C13 | 177.27 (9)  |
|-----------------|--------------|-----------------|-------------|
| C2—C1—C5—C9     | 174.88 (12)  | C18—C14—Si2—C13 | -65.49 (10) |
| Si1—C1—C5—C9    | -65.38 (14)  | C15—C14—Si2—Si1 | -60.65 (9)  |
| C18—C14—C15—C16 | -3.64(13)    | C18—C14—Si2—Si1 | 56.59 (9)   |
| Si2—C14—C15—C16 | 119.27 (10)  | C11—Si1—Si2—C12 | -178.64 (6) |
| C18—C14—C15—C19 | 175.62 (11)  | C10—Si1—Si2—C12 | -61.77 (7)  |
| Si2—C14—C15—C19 | -61.48 (14)  | C1—Si1—Si2—C12  | 59.96 (6)   |
| C19—C15—C16—C17 | -176.98 (12) | C11—Si1—Si2—C13 | 62.88 (7)   |
| C14—C15—C16—C17 | 2.25 (14)    | C10—Si1—Si2—C13 | 179.74 (6)  |
| C19—C15—C16—C20 | 0.9(2)       | C1—Si1—Si2—C13  | -58.52 (6)  |
| C14—C15—C16—C20 | -179.88 (12) | C11—Si1—Si2—C14 | -57.68 (6)  |
| C15—C16—C17—C18 | 0.24 (14)    | C10—Si1—Si2—C14 | 59.19 (6)   |
| C20—C16—C17—C18 | -177.76 (12) | C1—Si1—Si2—C14  | -179.08(5)  |
| C15—C16—C17—C21 | 177.99 (12)  |                 |             |

#### Hydrogen-bond geometry (Å, $^{o}$ )

Cg1 is the centroid of the C15–C18 ring.

| D— $H$ ··· $A$                    | D—H  | $H\cdots A$ | D··· $A$ | D— $H$ ··· $A$ |
|-----------------------------------|------|-------------|----------|----------------|
| C1—H1··· <i>Cg</i> 1 <sup>i</sup> | 1.00 | 2.65        | 3.646    | 173            |

Symmetry code: (i) -x+3/2, y-1/2, -z+1/2.