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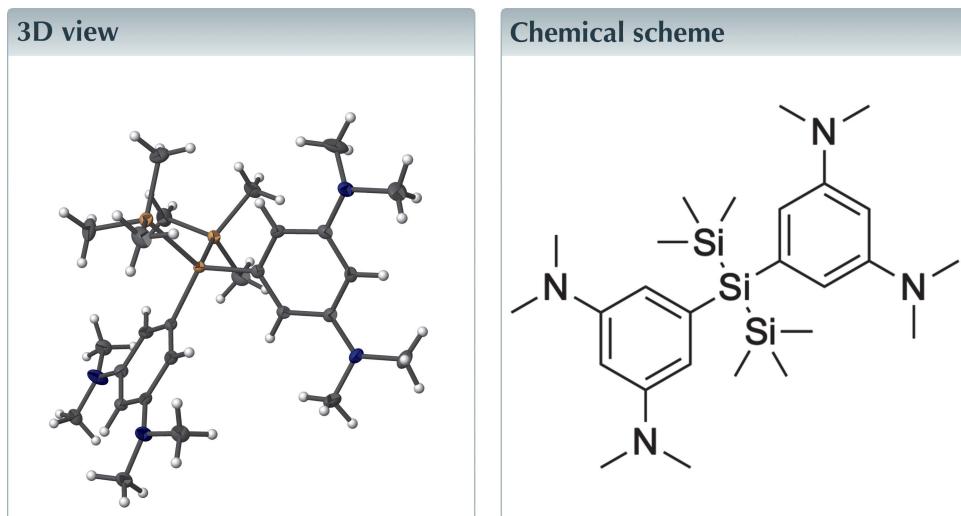
Structural data: full structural data are available from iucrdata.iucr.org

2,2-Bis[3,5-bis(dimethylamino)phenyl]-1,1,1,3,3-hexamethyltrisilane

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The title compound, $C_{26}H_{48}N_4Si_3$, was synthesized by the reaction of 2,2-dichlorotrisilane with 3,5-bis(dimethylamino)phenyllithium. In the molecule, the dihedral angle between the benzene rings is $57.57(7)^\circ$ and the Si—Si—Si bond angle is $110.08(2)^\circ$. In the crystal, molecules are linked via an SiC—H $\cdots\pi$ (aryl) interaction, forming a chain along the *c*-axis direction.



Structure description

Trisilane derivatives are often used as a precursor for divalent silicon compounds (silylenes) (Gaspar & West, 1998). Photoirradiation of a trisilane results in the elimination of a disilane derived from the silyl moieties of the both ends and the generation of a silylene from the central one. Silylenes are highly reactive and known to give the dimer, silicon–silicon double-bond compound (disilene) (West *et al.*, 1981), or higher oligomers without trapping reagent. Herein, we describe the synthesis and structural characterization of a novel trisilane bearing two 3,5-bis(dimethylamino)phenyl substituents on the central silicon atom.

In the molecule (Fig. 1), the Si—Si bond lengths are 2.3488 (5) and 2.3465 (5) Å, which are close to the shortest bond lengths among those of the reported 2,2-diaryl-1,1,1,3,3-hexamethyltrisilanes (2.347–2.397 Å; Archibald *et al.*, 1993; Lange *et al.*, 1991; Millevolte *et al.*, 1997; Pusztai *et al.*, 2013). The sums of the angles around the nitrogen atoms (N1, N2, N3 and N4) are 353.8, 358.9, 344.6 and 350.5°, respectively, indicating that the geometries around the nitrogen atoms on one aryl substituent with N3/N4 are more pyramidalized than those on the other with N1/N2. In the crystal, molecules are linked by an SiC—H $\cdots\pi$ (aryl) interaction (Fig. 2 and Table 1).



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Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

C_g is the centroid of the C14–C19 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C2–H4 \cdots C_g^i	0.98	2.81	3.7869 (17)	172

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

Synthesis and crystallization

To a solution of 1-bromo-3,5-bis(dimethylamino)benzene (194.6 mg, 0.80 mmol) in Et_2O (6.0 ml) was added *t*-BuLi (1.64 *M* in pentane, 1.07 ml, 1.76 mmol) at $-78\text{ }^\circ\text{C}$, and the solution was stirred for 1 h at the same temperature. Then, 2,2-dichloro-1,1,1,3,3,3-hexamethyltrisilane (104.2 mg, 0.42 mmol) in Et_2O (4 ml) was added dropwise, and the reaction mixture was gradually warmed up to room temperature over 14 h. After quenching with a saturated aqueous solution of NH_4Cl (10 ml), the water phase was extracted with Et_2O (10 ml \times 2). The combined organic phase was dried over Na_2SO_4 and evaporated *in vacuo*. Finally, recrystallization from the mixed solvents of hexane/dichloromethane gave the title compound (101.3 mg, 0.21 mmol, 50%) as colorless crystals. ^1H NMR (300 Hz, CDCl_3) δ 6.40 (*d*, $J = 1.2\text{ Hz}$, 4H), 6.11 (*t*, $J = 1.2\text{ Hz}$, 2H), 2.90 (*s*, 24H), 0.19 (*s*, 18H); ^{13}C NMR (75.5 Hz, CDCl_3) δ 151.1 (CH), 136.7 (C), 110.9 (CH), 98.6 (C), 41.1 (NCH₃), –0.012 (SiCH₃).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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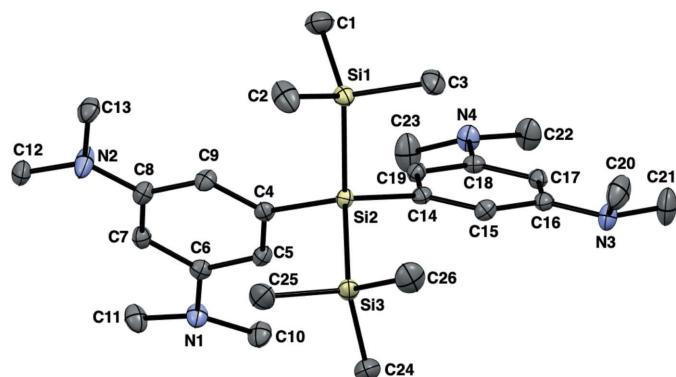


Figure 1

The molecular structure of the title compound, showing displacement ellipsoids at the 50% probability level. Hydrogen atoms are omitted for clarity.

Table 2
Experimental details.

Crystal data	
Chemical formula	$\text{C}_{26}\text{H}_{48}\text{N}_4\text{Si}_3$
M_r	500.95
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	103
a, b, c (\AA)	20.6543 (3), 8.3650 (1), 17.5215 (3)
β ($^\circ$)	97.371 (2)
V (\AA^3)	3002.23 (8)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.18
Crystal size (mm)	0.20 \times 0.20 \times 0.20
Data collection	
Diffractometer	Rigaku Saturn
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> (Rigaku OD, 2018))
T_{\min}, T_{\max}	0.977, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33409, 5581, 4877
R_{int}	0.029
($\sin \theta/\lambda$) _{max} (\AA^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.086, 1.04
No. of reflections	5581
No. of parameters	312
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ ($e\text{\AA}^{-3}$)	0.38, –0.18

Computer programs: *CrystalClear* (Rigaku, 1999), *CrysAlis PRO* (Rigaku OD, 2018), *SHELXT* (Sheldrick, 2015a), *SHELXL2018/I* (Sheldrick, 2015b), *Yadokari-XG* (Kabuto *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2020).

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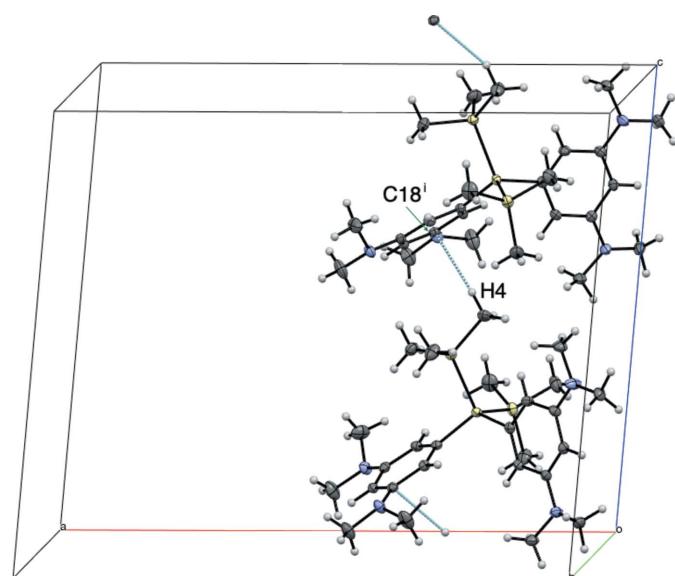


Figure 2

A packing diagram of the title compound, emphasizing the intermolecular SiC–H... π (aryl) interactions (light-blue dotted lines). [Symmetry code: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$].

computation time, which was provided by the Super Computer System (ICR, Kyoto University).

References

- Archibald, R. S., van den Winkel, Y., Powell, D. R. & West, R. (1993). *J. Organomet. Chem.* **446**, 67–72.
- Gaspar, P. P. & West, R. (1998). *The Chemistry of Organic Silicon Compounds*, Vol. 2, pp. 2463–2568. Chichester, UK: John Wiley & Sons, Ltd.
- Kabuto, C., Akine, S., Nemoto, T. & Kwon, E. (2009). *J. Crystallogr. Soc. Japan*, **51**, 218–224.
- Lange, L. D., Corey, J. Y. & Rath, N. P. (1991). *Organometallics*, **10**, 3189–3196.
- Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
- Millevolte, A. J., van den Winkel, Y., Powell, D. R. & West, R. (1997). *Organometallics*, **16**, 5375–5376.
- Pusztai, E., Toulokhonova, I. S., Temple, N., Albright, H., Zakai, U. I., Guo, S., Guzei, I. A., Hu, R. & West, R. (2013). *Organometallics*, **32**, 2529–2535.
- Rigaku (1999). Crystal Clear. Rigaku Corporation, Tokyo, Japan.
- Rigaku OD (2018). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
- Sheldrick, G. M. (2015a). *Acta Cryst. A* **71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst. C* **71**, 3–8.
- West, R., Fink, M. J. & Michl, J. (1981). *Science*, **214**, 1343–1344.

full crystallographic data

IUCrData (2020). **5**, x201299 [https://doi.org/10.1107/S2414314620012997]

2,2-Bis[3,5-bis(dimethylamino)phenyl]-1,1,1,3,3-hexamethyltrisilane

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Crystal data

$C_{26}H_{48}N_4Si_3$
 $M_r = 500.95$
Monoclinic, $P2_1/c$
 $a = 20.6543$ (3) Å
 $b = 8.3650$ (1) Å
 $c = 17.5215$ (3) Å
 $\beta = 97.371$ (2)°
 $V = 3002.23$ (8) Å³
 $Z = 4$

$F(000) = 1096$
 $D_x = 1.108 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 24488 reflections
 $\theta = 1.8\text{--}30.3^\circ$
 $\mu = 0.18 \text{ mm}^{-1}$
 $T = 103 \text{ K}$
Prism, colorless
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku Saturn
diffractometer
Radiation source: fine-focus sealed X-ray tube
Graphite monochromator
Detector resolution: 28.5714 pixels mm⁻¹
 ω scans
Absorption correction: multi-scan
(CrysAlisPro (Rigaku OD, 2018)
 $T_{\min} = 0.977$, $T_{\max} = 1.000$

33409 measured reflections
5581 independent reflections
4877 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
 $\theta_{\max} = 25.5^\circ$, $\theta_{\min} = 2.0^\circ$
 $h = -25 \rightarrow 25$
 $k = -10 \rightarrow 10$
 $l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.086$
 $S = 1.04$
5581 reflections
312 parameters
0 restraints
Primary atom site location: dual

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 1.4907P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.38 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.18 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Si1	0.30425 (2)	0.26359 (5)	0.40578 (2)	0.01776 (11)
Si2	0.25081 (2)	0.23923 (4)	0.27966 (2)	0.01378 (10)
Si3	0.20713 (2)	-0.01864 (5)	0.26001 (2)	0.01934 (11)
C1	0.32187 (9)	0.4774 (2)	0.43281 (10)	0.0326 (4)
H1	0.342782	0.529781	0.392332	0.049*
H2	0.351105	0.481717	0.481460	0.049*
H3	0.280943	0.532430	0.438785	0.049*
C2	0.25745 (8)	0.1727 (2)	0.47983 (9)	0.0338 (4)
H4	0.282593	0.183946	0.530913	0.051*
H5	0.249861	0.059114	0.468290	0.051*
H6	0.215449	0.227615	0.478973	0.051*
C3	0.38414 (7)	0.1570 (2)	0.40627 (9)	0.0278 (4)
H7	0.409142	0.164627	0.457597	0.042*
H8	0.408976	0.206399	0.368441	0.042*
H9	0.376058	0.044327	0.393031	0.042*
C4	0.17831 (7)	0.37787 (16)	0.26124 (8)	0.0157 (3)
C5	0.15255 (7)	0.42232 (16)	0.18664 (8)	0.0166 (3)
H10	0.174097	0.391031	0.144264	0.020*
C6	0.09489 (7)	0.51314 (16)	0.17395 (8)	0.0164 (3)
C7	0.06416 (7)	0.55949 (17)	0.23737 (8)	0.0175 (3)
H11	0.025674	0.622675	0.229263	0.021*
C8	0.08913 (7)	0.51440 (17)	0.31244 (8)	0.0189 (3)
C9	0.14687 (7)	0.42416 (17)	0.32341 (8)	0.0181 (3)
H12	0.164780	0.394190	0.374040	0.022*
N1	0.06746 (6)	0.55413 (15)	0.09955 (7)	0.0211 (3)
C10	0.10803 (8)	0.5412 (2)	0.03772 (8)	0.0247 (3)
H13	0.120610	0.429339	0.031923	0.037*
H14	0.147335	0.606661	0.050088	0.037*
H15	0.083461	0.578969	-0.010478	0.037*
C11	0.01575 (7)	0.6719 (2)	0.08958 (9)	0.0252 (3)
H16	0.032046	0.773793	0.112060	0.038*
H17	-0.020940	0.635214	0.115365	0.038*
H18	0.001115	0.686560	0.034579	0.038*
N2	0.05745 (7)	0.55862 (18)	0.37463 (7)	0.0305 (3)
C12	0.00044 (7)	0.65851 (19)	0.36342 (9)	0.0235 (3)
H19	-0.032513	0.609127	0.325453	0.035*
H20	0.012242	0.763704	0.344817	0.035*
H21	-0.017287	0.670837	0.412357	0.035*
C13	0.08889 (8)	0.5299 (2)	0.45176 (8)	0.0253 (3)
H22	0.131207	0.584552	0.459169	0.038*
H23	0.095511	0.414821	0.459639	0.038*
H24	0.061305	0.570997	0.488874	0.038*
C14	0.31425 (7)	0.28489 (17)	0.21410 (8)	0.0151 (3)
C15	0.35872 (7)	0.16651 (17)	0.19910 (8)	0.0170 (3)
H25	0.353827	0.060958	0.217532	0.020*

C16	0.41035 (7)	0.20138 (17)	0.15730 (8)	0.0169 (3)
C17	0.41619 (7)	0.35685 (17)	0.12925 (8)	0.0167 (3)
H26	0.450754	0.381126	0.100236	0.020*
C18	0.37191 (7)	0.47750 (17)	0.14323 (8)	0.0162 (3)
C19	0.32122 (7)	0.43937 (17)	0.18636 (8)	0.0160 (3)
H27	0.291203	0.520064	0.196795	0.019*
N3	0.45454 (6)	0.07908 (15)	0.14290 (7)	0.0215 (3)
N4	0.37992 (6)	0.63483 (15)	0.11844 (7)	0.0219 (3)
C20	0.47693 (9)	-0.0230 (2)	0.20856 (10)	0.0358 (4)
H28	0.439219	-0.073086	0.227626	0.054*
H29	0.500814	0.041608	0.249542	0.054*
H30	0.505801	-0.106202	0.192602	0.054*
C21	0.50722 (8)	0.1230 (2)	0.09949 (11)	0.0366 (4)
H31	0.536208	0.199436	0.129305	0.055*
H32	0.488974	0.171889	0.050608	0.055*
H33	0.532024	0.027143	0.089272	0.055*
C22	0.43019 (8)	0.6685 (2)	0.07004 (10)	0.0313 (4)
H34	0.419445	0.614702	0.020332	0.047*
H35	0.472326	0.629362	0.095198	0.047*
H36	0.432763	0.784068	0.061867	0.047*
C23	0.32265 (9)	0.7339 (2)	0.10043 (12)	0.0361 (4)
H37	0.294343	0.722489	0.140908	0.054*
H38	0.298835	0.700536	0.051007	0.054*
H39	0.335941	0.845920	0.097152	0.054*
C24	0.18019 (8)	-0.0508 (2)	0.15471 (10)	0.0310 (4)
H40	0.146709	0.028127	0.136380	0.047*
H41	0.162104	-0.158697	0.146642	0.047*
H42	0.217687	-0.038664	0.126137	0.047*
C25	0.13399 (8)	-0.0289 (2)	0.31312 (10)	0.0332 (4)
H43	0.148027	-0.019567	0.368531	0.050*
H44	0.111634	-0.131258	0.302292	0.050*
H45	0.104091	0.058891	0.296305	0.050*
C26	0.26437 (9)	-0.18132 (19)	0.29957 (11)	0.0340 (4)
H46	0.242957	-0.285333	0.290345	0.051*
H47	0.276191	-0.165481	0.355026	0.051*
H48	0.303862	-0.178120	0.274009	0.051*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0165 (2)	0.0216 (2)	0.0150 (2)	-0.00027 (16)	0.00150 (15)	0.00142 (15)
Si2	0.01451 (19)	0.01279 (19)	0.0143 (2)	0.00137 (14)	0.00278 (15)	0.00109 (14)
Si3	0.0186 (2)	0.0153 (2)	0.0246 (2)	-0.00180 (15)	0.00459 (16)	-0.00247 (16)
C1	0.0323 (9)	0.0292 (9)	0.0344 (9)	-0.0007 (7)	-0.0026 (7)	-0.0108 (7)
C2	0.0262 (9)	0.0523 (11)	0.0230 (8)	0.0001 (8)	0.0038 (7)	0.0145 (8)
C3	0.0216 (8)	0.0364 (9)	0.0241 (8)	0.0064 (7)	-0.0022 (6)	0.0008 (7)
C4	0.0161 (7)	0.0121 (7)	0.0191 (7)	-0.0007 (5)	0.0024 (5)	0.0003 (5)
C5	0.0185 (7)	0.0161 (7)	0.0161 (7)	0.0002 (6)	0.0055 (5)	-0.0011 (5)

C6	0.0174 (7)	0.0141 (7)	0.0174 (7)	-0.0013 (5)	0.0017 (5)	0.0016 (5)
C7	0.0161 (7)	0.0160 (7)	0.0205 (7)	0.0026 (5)	0.0031 (6)	0.0010 (6)
C8	0.0213 (7)	0.0179 (7)	0.0184 (7)	0.0018 (6)	0.0058 (6)	-0.0005 (6)
C9	0.0215 (7)	0.0187 (7)	0.0142 (7)	0.0025 (6)	0.0022 (6)	0.0020 (6)
N1	0.0211 (6)	0.0263 (7)	0.0160 (6)	0.0063 (5)	0.0023 (5)	0.0031 (5)
C10	0.0269 (8)	0.0313 (9)	0.0160 (7)	0.0049 (7)	0.0036 (6)	0.0021 (6)
C11	0.0208 (8)	0.0324 (9)	0.0221 (8)	0.0058 (7)	0.0017 (6)	0.0082 (7)
N2	0.0318 (8)	0.0440 (9)	0.0167 (7)	0.0209 (7)	0.0063 (6)	0.0012 (6)
C12	0.0197 (7)	0.0287 (8)	0.0234 (8)	0.0037 (6)	0.0076 (6)	-0.0035 (6)
C13	0.0286 (8)	0.0308 (9)	0.0174 (7)	0.0046 (7)	0.0065 (6)	-0.0015 (6)
C14	0.0162 (7)	0.0170 (7)	0.0120 (6)	-0.0003 (5)	0.0009 (5)	-0.0009 (5)
C15	0.0205 (7)	0.0139 (7)	0.0168 (7)	0.0003 (6)	0.0029 (6)	0.0012 (5)
C16	0.0165 (7)	0.0186 (7)	0.0151 (7)	0.0019 (6)	-0.0001 (5)	-0.0027 (6)
C17	0.0147 (7)	0.0210 (7)	0.0145 (7)	-0.0017 (6)	0.0026 (5)	-0.0009 (6)
C18	0.0179 (7)	0.0160 (7)	0.0143 (7)	-0.0020 (6)	0.0000 (5)	-0.0009 (5)
C19	0.0167 (7)	0.0150 (7)	0.0162 (7)	0.0017 (5)	0.0020 (5)	-0.0013 (5)
N3	0.0209 (6)	0.0216 (6)	0.0235 (7)	0.0063 (5)	0.0081 (5)	0.0010 (5)
N4	0.0241 (7)	0.0167 (6)	0.0263 (7)	-0.0010 (5)	0.0091 (5)	0.0041 (5)
C20	0.0400 (10)	0.0374 (10)	0.0298 (9)	0.0231 (8)	0.0042 (7)	0.0039 (8)
C21	0.0317 (9)	0.0311 (9)	0.0515 (11)	0.0105 (8)	0.0228 (8)	0.0035 (8)
C22	0.0336 (9)	0.0212 (8)	0.0424 (10)	-0.0047 (7)	0.0176 (8)	0.0052 (7)
C23	0.0356 (10)	0.0219 (8)	0.0543 (12)	0.0070 (7)	0.0190 (9)	0.0157 (8)
C24	0.0274 (9)	0.0335 (9)	0.0315 (9)	0.0003 (7)	0.0012 (7)	-0.0130 (7)
C25	0.0278 (9)	0.0335 (9)	0.0405 (10)	-0.0119 (7)	0.0129 (7)	-0.0069 (8)
C26	0.0376 (10)	0.0169 (8)	0.0474 (11)	0.0013 (7)	0.0056 (8)	0.0039 (7)

Geometric parameters (\AA , ^\circ)

Si1—C1	1.8737 (17)	C12—H20	0.9800
Si1—C3	1.8744 (16)	C12—H21	0.9800
Si1—C2	1.8755 (16)	C13—H22	0.9800
Si1—Si2	2.3488 (5)	C13—H23	0.9800
Si2—C4	1.8887 (14)	C13—H24	0.9800
Si2—C14	1.8890 (14)	C14—C19	1.395 (2)
Si2—Si3	2.3465 (5)	C14—C15	1.398 (2)
Si3—C25	1.8751 (17)	C15—C16	1.400 (2)
Si3—C26	1.8762 (17)	C15—H25	0.9500
Si3—C24	1.8767 (17)	C16—C17	1.401 (2)
C1—H1	0.9800	C16—N3	1.4151 (18)
C1—H2	0.9800	C17—C18	1.404 (2)
C1—H3	0.9800	C17—H26	0.9500
C2—H4	0.9800	C18—N4	1.4023 (18)
C2—H5	0.9800	C18—C19	1.404 (2)
C2—H6	0.9800	C19—H27	0.9500
C3—H7	0.9800	N3—C21	1.452 (2)
C3—H8	0.9800	N3—C20	1.460 (2)
C3—H9	0.9800	N4—C23	1.446 (2)
C4—C9	1.393 (2)	N4—C22	1.4499 (19)

C4—C5	1.3971 (19)	C20—H28	0.9800
C5—C6	1.406 (2)	C20—H29	0.9800
C5—H10	0.9500	C20—H30	0.9800
C6—N1	1.3959 (18)	C21—H31	0.9800
C6—C7	1.403 (2)	C21—H32	0.9800
C7—C8	1.402 (2)	C21—H33	0.9800
C7—H11	0.9500	C22—H34	0.9800
C8—N2	1.3911 (19)	C22—H35	0.9800
C8—C9	1.404 (2)	C22—H36	0.9800
C9—H12	0.9500	C23—H37	0.9800
N1—C11	1.4473 (19)	C23—H38	0.9800
N1—C10	1.4562 (19)	C23—H39	0.9800
C10—H13	0.9800	C24—H40	0.9800
C10—H14	0.9800	C24—H41	0.9800
C10—H15	0.9800	C24—H42	0.9800
C11—H16	0.9800	C25—H43	0.9800
C11—H17	0.9800	C25—H44	0.9800
C11—H18	0.9800	C25—H45	0.9800
N2—C12	1.4365 (19)	C26—H46	0.9800
N2—C13	1.4423 (19)	C26—H47	0.9800
C12—H19	0.9800	C26—H48	0.9800
C1—Si1—C3	108.08 (8)	N2—C12—H21	109.5
C1—Si1—C2	108.21 (9)	H19—C12—H21	109.5
C3—Si1—C2	109.61 (8)	H20—C12—H21	109.5
C1—Si1—Si2	111.92 (6)	N2—C13—H22	109.5
C3—Si1—Si2	105.68 (5)	N2—C13—H23	109.5
C2—Si1—Si2	113.20 (6)	H22—C13—H23	109.5
C4—Si2—C14	111.62 (6)	N2—C13—H24	109.5
C4—Si2—Si3	104.95 (4)	H22—C13—H24	109.5
C14—Si2—Si3	112.35 (5)	H23—C13—H24	109.5
C4—Si2—Si1	111.97 (5)	C19—C14—C15	119.40 (13)
C14—Si2—Si1	106.00 (4)	C19—C14—Si2	120.66 (10)
Si3—Si2—Si1	110.08 (2)	C15—C14—Si2	119.65 (10)
C25—Si3—C26	107.05 (8)	C14—C15—C16	120.91 (13)
C25—Si3—C24	108.98 (8)	C14—C15—H25	119.5
C26—Si3—C24	110.64 (8)	C16—C15—H25	119.5
C25—Si3—Si2	106.75 (6)	C15—C16—C17	118.86 (13)
C26—Si3—Si2	113.60 (6)	C15—C16—N3	119.66 (13)
C24—Si3—Si2	109.63 (6)	C17—C16—N3	121.47 (13)
Si1—C1—H1	109.5	C16—C17—C18	121.24 (13)
Si1—C1—H2	109.5	C16—C17—H26	119.4
H1—C1—H2	109.5	C18—C17—H26	119.4
Si1—C1—H3	109.5	N4—C18—C19	120.37 (13)
H1—C1—H3	109.5	N4—C18—C17	121.00 (13)
H2—C1—H3	109.5	C19—C18—C17	118.54 (13)
Si1—C2—H4	109.5	C14—C19—C18	121.03 (13)
Si1—C2—H5	109.5	C14—C19—H27	119.5

H4—C2—H5	109.5	C18—C19—H27	119.5
Si1—C2—H6	109.5	C16—N3—C21	117.02 (12)
H4—C2—H6	109.5	C16—N3—C20	115.40 (12)
H5—C2—H6	109.5	C21—N3—C20	112.20 (13)
Si1—C3—H7	109.5	C18—N4—C23	118.68 (12)
Si1—C3—H8	109.5	C18—N4—C22	119.02 (12)
H7—C3—H8	109.5	C23—N4—C22	112.84 (13)
Si1—C3—H9	109.5	N3—C20—H28	109.5
H7—C3—H9	109.5	N3—C20—H29	109.5
H8—C3—H9	109.5	H28—C20—H29	109.5
C9—C4—C5	119.86 (13)	N3—C20—H30	109.5
C9—C4—Si2	118.43 (10)	H28—C20—H30	109.5
C5—C4—Si2	121.45 (11)	H29—C20—H30	109.5
C4—C5—C6	120.33 (13)	N3—C21—H31	109.5
C4—C5—H10	119.8	N3—C21—H32	109.5
C6—C5—H10	119.8	H31—C21—H32	109.5
N1—C6—C7	120.08 (13)	N3—C21—H33	109.5
N1—C6—C5	120.96 (13)	H31—C21—H33	109.5
C7—C6—C5	118.95 (13)	H32—C21—H33	109.5
C8—C7—C6	121.30 (13)	N4—C22—H34	109.5
C8—C7—H11	119.4	N4—C22—H35	109.5
C6—C7—H11	119.4	H34—C22—H35	109.5
N2—C8—C7	120.67 (13)	N4—C22—H36	109.5
N2—C8—C9	120.83 (13)	H34—C22—H36	109.5
C7—C8—C9	118.50 (13)	H35—C22—H36	109.5
C4—C9—C8	121.05 (13)	N4—C23—H37	109.5
C4—C9—H12	119.5	N4—C23—H38	109.5
C8—C9—H12	119.5	H37—C23—H38	109.5
C6—N1—C11	118.99 (12)	N4—C23—H39	109.5
C6—N1—C10	118.25 (12)	H37—C23—H39	109.5
C11—N1—C10	116.55 (12)	H38—C23—H39	109.5
N1—C10—H13	109.5	Si3—C24—H40	109.5
N1—C10—H14	109.5	Si3—C24—H41	109.5
H13—C10—H14	109.5	H40—C24—H41	109.5
N1—C10—H15	109.5	Si3—C24—H42	109.5
H13—C10—H15	109.5	H40—C24—H42	109.5
H14—C10—H15	109.5	H41—C24—H42	109.5
N1—C11—H16	109.5	Si3—C25—H43	109.5
N1—C11—H17	109.5	Si3—C25—H44	109.5
H16—C11—H17	109.5	H43—C25—H44	109.5
N1—C11—H18	109.5	Si3—C25—H45	109.5
H16—C11—H18	109.5	H43—C25—H45	109.5
H17—C11—H18	109.5	H44—C25—H45	109.5
C8—N2—C12	120.48 (12)	Si3—C26—H46	109.5
C8—N2—C13	119.29 (12)	Si3—C26—H47	109.5
C12—N2—C13	119.17 (12)	H46—C26—H47	109.5
N2—C12—H19	109.5	Si3—C26—H48	109.5
N2—C12—H20	109.5	H46—C26—H48	109.5

H19—C12—H20	109.5	H47—C26—H48	109.5
C14—Si2—C4—C9	−145.45 (11)	C4—Si2—C14—C19	28.69 (13)
Si3—Si2—C4—C9	92.60 (11)	Si3—Si2—C14—C19	146.27 (10)
Si1—Si2—C4—C9	−26.80 (12)	Si1—Si2—C14—C19	−93.46 (11)
C14—Si2—C4—C5	40.35 (13)	C4—Si2—C14—C15	−157.41 (11)
Si3—Si2—C4—C5	−81.60 (12)	Si3—Si2—C14—C15	−39.83 (12)
Si1—Si2—C4—C5	159.00 (10)	Si1—Si2—C14—C15	80.44 (11)
C9—C4—C5—C6	−0.2 (2)	C19—C14—C15—C16	0.6 (2)
Si2—C4—C5—C6	173.90 (10)	Si2—C14—C15—C16	−173.39 (10)
C4—C5—C6—N1	−177.96 (13)	C14—C15—C16—C17	−1.2 (2)
C4—C5—C6—C7	0.6 (2)	C14—C15—C16—N3	−179.91 (12)
N1—C6—C7—C8	177.34 (13)	C15—C16—C17—C18	0.8 (2)
C5—C6—C7—C8	−1.3 (2)	N3—C16—C17—C18	179.53 (12)
C6—C7—C8—N2	−178.75 (14)	C16—C17—C18—N4	176.69 (13)
C6—C7—C8—C9	1.4 (2)	C16—C17—C18—C19	0.1 (2)
C5—C4—C9—C8	0.4 (2)	C15—C14—C19—C18	0.4 (2)
Si2—C4—C9—C8	−173.87 (11)	Si2—C14—C19—C18	174.32 (10)
N2—C8—C9—C4	179.17 (14)	N4—C18—C19—C14	−177.34 (13)
C7—C8—C9—C4	−1.0 (2)	C17—C18—C19—C14	−0.7 (2)
C7—C6—N1—C11	13.1 (2)	C15—C16—N3—C21	−179.75 (14)
C5—C6—N1—C11	−168.37 (13)	C17—C16—N3—C21	1.6 (2)
C7—C6—N1—C10	164.45 (13)	C15—C16—N3—C20	−44.38 (19)
C5—C6—N1—C10	−17.0 (2)	C17—C16—N3—C20	136.94 (15)
C7—C8—N2—C12	−3.3 (2)	C19—C18—N4—C23	−32.2 (2)
C9—C8—N2—C12	176.48 (14)	C17—C18—N4—C23	151.30 (15)
C7—C8—N2—C13	−171.42 (14)	C19—C18—N4—C22	−176.24 (13)
C9—C8—N2—C13	8.4 (2)	C17—C18—N4—C22	7.3 (2)

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the C14—C19 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H4···Cg ⁱ	0.98	2.81	3.7869 (17)	172

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