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N-[1-Phenyl-2,5-bis(trimethylsilyl)pent-2-en-4-yn-1-yl]aniline

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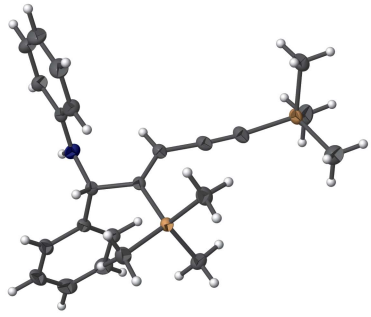
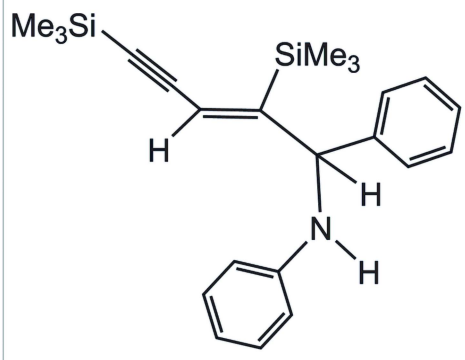
The molecular structure of the title compound, $C_{23}H_{31}NSi_2$, reveals an acyclic conjugated enyne unit as the main feature. The central pent-2-en-4-yl fragment is essentially planar, with a maximum deviation of 0.0492 (7) Å from the mean plane defined by the C—C=C—C≡C unit. The dihedral angle between the phenyl rings is 84.44 (5)°.

3D view



Chemical scheme



Structure description

Compounds that contain conjugated enyne fragments are valuable building blocks in organic synthesis, since these are important units in medicinal and material science (Ochiai *et al.*, 1999; Saito *et al.*, 2001). The title compound (Fig. 1) was synthesized by hydrolysis of the corresponding zirconocene aza-metallacycle in toluene. The observed bond lengths and angles of the central acyclic amino-pent-2-en-4-yl fragment [C1—C2 1.2048 (17), C2—C3 1.4325 (16), C3—C4 1.3448 (15) Å; C1—C2—C3 175.03 (13), C2—C3—C4 126.26 (12)°] are comparable with those of similar derivatives with acyclic pent-2-en-4-yn-amides (Feng *et al.*, 2014; Li *et al.*, 2014; Meng & Wan, 2013; Cheng *et al.*, 2012; Borbulevych *et al.*, 1999, 2001), a polymer containing [$(Ph)_2N—CH_2—C{=}C—C{\equiv}C$–] building blocks (Enkelmann & Schleier, 1980) and an ammonium salt (Kuminek *et al.*, 2013; Tedesco *et al.*, 2002). As expected, the central pent-2-en-4-yl fragment of the title compound is nearly planar; mean deviation of the best plane defined by C1, C2, C3, C4 and C5 is 0.037 Å. The observed dihedral angle between the phenyl rings is 84.44 (5)°.

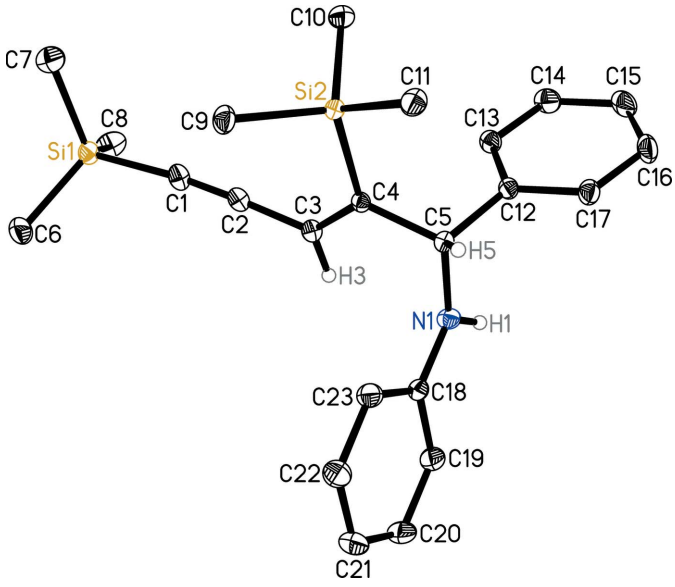


Figure 1
Molecular structure of the title compound with atom labelling and displacement ellipsoids drawn at the 30% probability level. For clarity H atoms except H1, H3 and H5 have been omitted.

Synthesis and crystallization

All manipulations were carried out under an argon atmosphere using standard Schlenk techniques. Toluene and *n*-hexane were dried over two columns with activated aluminium oxide with an Inert PureSolv MD5 solvent purification system (Innovative Technology). To a dark-red toluene solution (10 ml) of bis(cyclopentadienyl){*N*-[1-phenyl-2,5-bis(trimethylsilyl)pent-2-en-4-yn-1-yl]anilido}zirconium (0.242 g, 0.405 mmol), which was prepared according to the method of Burlakov *et al.* (2014), was added 8.5 ml of water saturated toluene and the resulting mixture was kept at room temperature without stirring. After one day, the light-yellow solution had evaporated to dryness. The residue was extracted with 10 ml of *n*-hexane. The colourless solution was filtered, concentrated to 1–1.5 ml and allowed to stand at room temperature. After one day, colourless crystals were separated from the mother liquor, washed with cold *n*-hexane, and dried in vacuum to give 0.088 g (58%) of the title compound. Single crystals were obtained from a saturated solution dissolved in *n*-hexane at room temperature.

M.p.: 99–100°C under Ar. Elemental analysis: calculated for $C_{23}H_{31}NSi_2$: C 73.14, H 8.27, N 3.71%; found: C 72.83, H 8.02, N 3.50%. IR (ATR, cm^{-1}): 2125, 2182 (C≡C), 3401(N—H). MS (70 eV, *m*/*z*): 377 $[M]^+$, 304 $[M - SiMe_3]^+$, 197 $[Me_3SiC_2—CH{=}CH—SiMe_3 + H]^+$, 182 $[PhN{=}CHPh + H]^+$, 73 $[SiMe_3]^+$.

^{1}H NMR (300 MHz, C_6D_6, 297 K): δ (p.p.m.) 0.19 (*s*, 9H, $SiMe_3$); 0.29 (*s*, 9H, $SiMe_3$); 3.50 (*d*, 1H, NH); 5.07 (*d*, 1H, CHPh); 6.38 (*m*, 2H, *o*-Ph); 6.52 (*s*, 1H, CH═C); 6.69 (*m*, 1H, *p*-Ph) 7.03–7.11 (*m*, 7H, Ph). **^{13}C NMR** (75 MHz, C_6D_6, 297 K): δ (p.p.m.) −0.9, −0.3 ($SiMe_3$); 63.1 (CHPh); 101.5, 105.7 (C≡C); 113.6 (*o*,*m*-Ph); 118.1, 121.3 (*p*-Ph); 127.9 (CH═C); 128.8, 128.8, 129.5 (*o*,*m*-Ph); 141.2, 147.1 (*i*-Ph); 156.8 (CH═C).

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{31}NSi_2$
M_r	377.67
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, *b*, *c* (Å)	11.0662 (5), 11.1661 (5), 11.2508 (5)
α, β, γ (°)	65.2268 (6), 67.0573 (6), 71.9789 (6)
V (Å^3)	1144.57 (9)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.16
Crystal size (mm)	0.46 × 0.31 × 0.31
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.93, 0.95
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22773, 5526, 4641
R_{int}	0.026
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.660
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.032, 0.086, 1.03
No. of reflections	5526
No. of parameters	245
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.20

Computer programs: *APEX2* (Bruker, 2011), *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *XP* in *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

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full crystallographic data

IUCrData (2016). **1**, x161559 [https://doi.org/10.1107/S2414314616015595]

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Crystal data

$C_{23}H_{31}NSi_2$
M_r = 377.67
Triclinic, $P\overline{1}$
a = 11.0662 (5) Å
b = 11.1661 (5) Å
c = 11.2508 (5) Å
α = 65.2268 (6)°
β = 67.0573 (6)°
γ = 71.9789 (6)°
V = 1144.57 (9) Å^3
Z = 2
$F(000)$ = 408
D_x = 1.096 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9956 reflections
θ = 2.4–28.8°
μ = 0.16 mm^{-1}
T = 150 K
Prism, pale yellow
0.46 × 0.31 × 0.31 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2008)
T_{min} = 0.93, T_{max} = 0.95
22773 measured reflections
5526 independent reflections
4641 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 28.0°, θ_{min} = 2.0°
h = −14→14
k = −14→14
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.086
S = 1.03
5526 reflections
245 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0362P)^2 + 0.4111P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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}*/U_{eq}
C1	0.74405 (12)	0.65953 (14)	0.53612 (12)	0.0277 (3)
C2	0.70399 (11)	0.63622 (13)	0.46400 (11)	0.0242 (2)
C3	0.65238 (11)	0.59872 (12)	0.38833 (11)	0.0223 (2)
H3	0.6319	0.5110	0.4276	0.027*
C4	0.63021 (10)	0.67573 (11)	0.26706 (11)	0.0181 (2)
C5	0.56351 (11)	0.62132 (11)	0.20861 (11)	0.0189 (2)
H5	0.6128	0.6409	0.1086	0.023*
C6	0.97016 (16)	0.55728 (17)	0.65491 (18)	0.0444 (4)
H6A	0.9518	0.4662	0.6896	0.067*
H6B	1.0089	0.5657	0.7154	0.067*
H6C	1.0331	0.5754	0.5620	0.067*
C7	0.84118 (16)	0.85404 (15)	0.58691 (16)	0.0405 (3)
H7A	0.8996	0.8762	0.4919	0.061*
H7B	0.8832	0.8624	0.6446	0.061*
H7C	0.7557	0.9156	0.5906	0.061*
C8	0.68621 (17)	0.64354 (17)	0.82272 (14)	0.0427 (4)
H8A	0.6046	0.7101	0.8176	0.064*
H8B	0.7211	0.6478	0.8884	0.064*
H8C	0.6662	0.5539	0.8530	0.064*
C9	0.84620 (12)	0.84738 (14)	0.15867 (14)	0.0300 (3)
H9A	0.9082	0.7767	0.1239	0.045*
H9B	0.8487	0.8302	0.2506	0.045*
H9C	0.8723	0.9343	0.0969	0.045*
C10	0.55181 (13)	0.96905 (14)	0.25251 (15)	0.0320 (3)
H10A	0.5759	1.0584	0.2024	0.048*
H10B	0.5532	0.9393	0.3473	0.048*
H10C	0.4622	0.9725	0.2526	0.048*
C11	0.66940 (14)	0.89749 (13)	−0.01128 (12)	0.0296 (3)
H11A	0.6802	0.9913	−0.0616	0.044*
H11B	0.5837	0.8862	−0.0083	0.044*
H11C	0.7419	0.8403	−0.0578	0.044*
C12	0.41890 (11)	0.69124 (12)	0.22133 (12)	0.0213 (2)
C13	0.34076 (12)	0.73615 (13)	0.33064 (13)	0.0258 (3)
H13	0.3789	0.7283	0.3966	0.031*
C14	0.20694 (13)	0.79257 (15)	0.34416 (16)	0.0351 (3)
H14	0.1541	0.8232	0.4191	0.042*
C15	0.15117 (13)	0.80401 (15)	0.24842 (17)	0.0396 (3)
H15	0.0598	0.8422	0.2579	0.048*
C16	0.22787 (14)	0.76003 (15)	0.13902 (16)	0.0378 (3)
H16	0.1893	0.7679	0.0735	0.045*
C17	0.36149 (13)	0.70431 (13)	0.12505 (13)	0.0282 (3)
H17	0.4142	0.6749	0.0493	0.034*
C18	0.67654 (12)	0.38337 (12)	0.24183 (12)	0.0229 (2)
C19	0.66529 (14)	0.24778 (13)	0.29765 (14)	0.0309 (3)
H19	0.5813	0.2219	0.3539	0.037*

C20	0.77569 (16)	0.15132 (15)	0.27136 (16)	0.0395 (3)
H20	0.7666	0.0597	0.3102	0.047*
C21	0.89939 (15)	0.18612 (16)	0.18919 (17)	0.0412 (3)
H21	0.9747	0.1193	0.1712	0.049*
C22	0.91101 (14)	0.31931 (15)	0.13411 (15)	0.0371 (3)
H22	0.9953	0.3442	0.0775	0.044*
C23	0.80156 (12)	0.41802 (14)	0.15989 (13)	0.0291 (3)
H23	0.8118	0.5093	0.1217	0.035*
N1	0.56481 (10)	0.47771 (10)	0.27120 (11)	0.0242 (2)
Si1	0.81276 (3)	0.67930 (4)	0.65053 (3)	0.02577 (9)
Si2	0.67391 (3)	0.84901 (3)	0.16732 (3)	0.01984 (8)
H1	0.4925 (16)	0.4510 (16)	0.3107 (16)	0.034 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0228 (6)	0.0382 (7)	0.0211 (5)	−0.0022 (5)	−0.0065 (5)	−0.0116 (5)
C2	0.0208 (5)	0.0291 (6)	0.0185 (5)	−0.0018 (5)	−0.0051 (4)	−0.0069 (5)
C3	0.0211 (5)	0.0248 (6)	0.0201 (5)	−0.0042 (4)	−0.0060 (4)	−0.0069 (5)
C4	0.0146 (5)	0.0212 (6)	0.0189 (5)	−0.0018 (4)	−0.0039 (4)	−0.0090 (4)
C5	0.0196 (5)	0.0202 (6)	0.0170 (5)	−0.0056 (4)	−0.0047 (4)	−0.0057 (4)
C6	0.0427 (8)	0.0459 (9)	0.0596 (10)	0.0066 (7)	−0.0325 (8)	−0.0262 (8)
C7	0.0422 (8)	0.0365 (8)	0.0416 (8)	−0.0083 (6)	−0.0097 (6)	−0.0139 (7)
C8	0.0617 (10)	0.0441 (9)	0.0233 (6)	−0.0158 (7)	−0.0046 (6)	−0.0153 (6)
C9	0.0237 (6)	0.0345 (7)	0.0348 (7)	−0.0100 (5)	−0.0094 (5)	−0.0107 (6)
C10	0.0314 (7)	0.0277 (7)	0.0405 (7)	−0.0007 (5)	−0.0122 (6)	−0.0171 (6)
C11	0.0390 (7)	0.0259 (7)	0.0247 (6)	−0.0123 (5)	−0.0130 (5)	−0.0018 (5)
C12	0.0205 (5)	0.0193 (6)	0.0237 (5)	−0.0070 (4)	−0.0084 (4)	−0.0028 (4)
C13	0.0210 (5)	0.0264 (6)	0.0287 (6)	−0.0057 (5)	−0.0067 (5)	−0.0076 (5)
C14	0.0210 (6)	0.0335 (7)	0.0467 (8)	−0.0048 (5)	−0.0048 (5)	−0.0149 (6)
C15	0.0213 (6)	0.0341 (8)	0.0613 (9)	−0.0043 (5)	−0.0174 (6)	−0.0102 (7)
C16	0.0351 (7)	0.0344 (8)	0.0504 (8)	−0.0110 (6)	−0.0276 (7)	−0.0034 (6)
C17	0.0302 (6)	0.0273 (7)	0.0305 (6)	−0.0099 (5)	−0.0140 (5)	−0.0051 (5)
C18	0.0259 (6)	0.0232 (6)	0.0236 (5)	−0.0024 (5)	−0.0105 (5)	−0.0102 (5)
C19	0.0345 (7)	0.0254 (7)	0.0351 (7)	−0.0064 (5)	−0.0125 (5)	−0.0095 (5)
C20	0.0491 (9)	0.0228 (7)	0.0509 (9)	0.0003 (6)	−0.0226 (7)	−0.0143 (6)
C21	0.0382 (8)	0.0357 (8)	0.0544 (9)	0.0100 (6)	−0.0194 (7)	−0.0262 (7)
C22	0.0263 (6)	0.0423 (8)	0.0445 (8)	−0.0010 (6)	−0.0068 (6)	−0.0237 (7)
C23	0.0269 (6)	0.0271 (7)	0.0333 (6)	−0.0045 (5)	−0.0068 (5)	−0.0126 (5)
N1	0.0206 (5)	0.0204 (5)	0.0295 (5)	−0.0066 (4)	−0.0033 (4)	−0.0082 (4)
Si1	0.02876 (18)	0.0307 (2)	0.02222 (16)	−0.00232 (14)	−0.01080 (13)	−0.01223 (14)
Si2	0.01964 (15)	0.01973 (17)	0.02223 (15)	−0.00389 (12)	−0.00781 (12)	−0.00738 (12)

Geometric parameters (Å, º)

C1—C2	1.2048 (17)	C10—H10C	0.9800
C1—Si1	1.8408 (13)	C11—Si2	1.8664 (13)
C2—C3	1.4325 (16)	C11—H11A	0.9800

C3—C4	1.3448 (15)	C11—H11B	0.9800
C3—H3	0.9500	C11—H11C	0.9800
C4—C5	1.5288 (15)	C12—C13	1.3897 (17)
C4—Si2	1.8903 (12)	C12—C17	1.3945 (16)
C5—N1	1.4543 (15)	C13—C14	1.3930 (17)
C5—C12	1.5274 (15)	C13—H13	0.9500
C5—H5	1.0000	C14—C15	1.383 (2)
C6—Si1	1.8534 (15)	C14—H14	0.9500
C6—H6A	0.9800	C15—C16	1.382 (2)
C6—H6B	0.9800	C15—H15	0.9500
C6—H6C	0.9800	C16—C17	1.3892 (19)
C7—Si1	1.8579 (16)	C16—H16	0.9500
C7—H7A	0.9800	C17—H17	0.9500
C7—H7B	0.9800	C18—N1	1.3838 (15)
C7—H7C	0.9800	C18—C23	1.3970 (17)
C8—Si1	1.8591 (15)	C18—C19	1.4004 (18)
C8—H8A	0.9800	C19—C20	1.382 (2)
C8—H8B	0.9800	C19—H19	0.9500
C8—H8C	0.9800	C20—C21	1.386 (2)
C9—Si2	1.8656 (12)	C20—H20	0.9500
C9—H9A	0.9800	C21—C22	1.377 (2)
C9—H9B	0.9800	C21—H21	0.9500
C9—H9C	0.9800	C22—C23	1.3907 (19)
C10—Si2	1.8675 (13)	C22—H22	0.9500
C10—H10A	0.9800	C23—H23	0.9500
C10—H10B	0.9800	N1—H1	0.829 (16)

C2—C1—Si1	174.85 (12)	C13—C12—C5	121.57 (10)
C1—C2—C3	175.03 (13)	C17—C12—C5	119.36 (11)
C4—C3—C2	126.26 (12)	C12—C13—C14	120.44 (12)
C4—C3—H3	116.9	C12—C13—H13	119.8
C2—C3—H3	116.9	C14—C13—H13	119.8
C3—C4—C5	118.20 (10)	C15—C14—C13	119.92 (13)
C3—C4—Si2	123.35 (9)	C15—C14—H14	120.0
C5—C4—Si2	118.43 (8)	C13—C14—H14	120.0
N1—C5—C12	107.86 (9)	C16—C15—C14	120.23 (12)
N1—C5—C4	114.45 (9)	C16—C15—H15	119.9
C12—C5—C4	111.42 (9)	C14—C15—H15	119.9
N1—C5—H5	107.6	C15—C16—C17	119.92 (13)
C12—C5—H5	107.6	C15—C16—H16	120.0
C4—C5—H5	107.6	C17—C16—H16	120.0
Si1—C6—H6A	109.5	C16—C17—C12	120.51 (13)
Si1—C6—H6B	109.5	C16—C17—H17	119.7
H6A—C6—H6B	109.5	C12—C17—H17	119.7
Si1—C6—H6C	109.5	N1—C18—C23	122.40 (11)
H6A—C6—H6C	109.5	N1—C18—C19	119.22 (11)
H6B—C6—H6C	109.5	C23—C18—C19	118.38 (12)
Si1—C7—H7A	109.5	C20—C19—C18	120.40 (13)

Si1—C7—H7B	109.5	C20—C19—H19	119.8
H7A—C7—H7B	109.5	C18—C19—H19	119.8
Si1—C7—H7C	109.5	C19—C20—C21	121.08 (14)
H7A—C7—H7C	109.5	C19—C20—H20	119.5
H7B—C7—H7C	109.5	C21—C20—H20	119.5
Si1—C8—H8A	109.5	C22—C21—C20	118.75 (13)
Si1—C8—H8B	109.5	C22—C21—H21	120.6
H8A—C8—H8B	109.5	C20—C21—H21	120.6
Si1—C8—H8C	109.5	C21—C22—C23	121.20 (13)
H8A—C8—H8C	109.5	C21—C22—H22	119.4
H8B—C8—H8C	109.5	C23—C22—H22	119.4
Si2—C9—H9A	109.5	C22—C23—C18	120.19 (13)
Si2—C9—H9B	109.5	C22—C23—H23	119.9
H9A—C9—H9B	109.5	C18—C23—H23	119.9
Si2—C9—H9C	109.5	C18—N1—C5	123.30 (10)
H9A—C9—H9C	109.5	C18—N1—H1	116.6 (11)
H9B—C9—H9C	109.5	C5—N1—H1	118.3 (11)
Si2—C10—H10A	109.5	C1—Si1—C6	107.81 (6)
Si2—C10—H10B	109.5	C1—Si1—C7	109.84 (7)
H10A—C10—H10B	109.5	C6—Si1—C7	111.43 (8)
Si2—C10—H10C	109.5	C1—Si1—C8	106.75 (7)
H10A—C10—H10C	109.5	C6—Si1—C8	111.28 (8)
H10B—C10—H10C	109.5	C7—Si1—C8	109.60 (7)
Si2—C11—H11A	109.5	C9—Si2—C11	108.21 (6)
Si2—C11—H11B	109.5	C9—Si2—C10	110.05 (6)
H11A—C11—H11B	109.5	C11—Si2—C10	111.04 (6)
Si2—C11—H11C	109.5	C9—Si2—C4	110.10 (6)
H11A—C11—H11C	109.5	C11—Si2—C4	107.97 (5)
H11B—C11—H11C	109.5	C10—Si2—C4	109.44 (6)
C13—C12—C17	118.98 (11)		

C2—C3—C4—C5	−174.92 (10)	N1—C18—C19—C20	−179.19 (12)
C2—C3—C4—Si2	3.72 (17)	C23—C18—C19—C20	−0.21 (19)
C3—C4—C5—N1	−16.43 (14)	C18—C19—C20—C21	−0.3 (2)
Si2—C4—C5—N1	164.86 (7)	C19—C20—C21—C22	0.3 (2)
C3—C4—C5—C12	106.27 (11)	C20—C21—C22—C23	0.2 (2)
Si2—C4—C5—C12	−72.45 (10)	C21—C22—C23—C18	−0.6 (2)
N1—C5—C12—C13	93.63 (13)	N1—C18—C23—C22	179.59 (12)
C4—C5—C12—C13	−32.78 (15)	C19—C18—C23—C22	0.65 (19)
N1—C5—C12—C17	−82.99 (13)	C23—C18—N1—C5	6.77 (18)
C4—C5—C12—C17	150.60 (11)	C19—C18—N1—C5	−174.29 (11)
C17—C12—C13—C14	0.39 (18)	C12—C5—N1—C18	158.89 (10)
C5—C12—C13—C14	−176.24 (11)	C4—C5—N1—C18	−76.51 (13)
C12—C13—C14—C15	0.1 (2)	C3—C4—Si2—C9	46.86 (11)
C13—C14—C15—C16	−0.2 (2)	C5—C4—Si2—C9	−134.49 (8)
C14—C15—C16—C17	−0.1 (2)	C3—C4—Si2—C11	164.81 (10)
C15—C16—C17—C12	0.5 (2)	C5—C4—Si2—C11	−16.55 (10)
C13—C12—C17—C16	−0.70 (19)	C3—C4—Si2—C10	−74.21 (11)

C5—C12—C17—C16	176.01 (11)	C5—C4—Si2—C10	104.43 (9)