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10-[1,1-Dichloro-4-(trimethylsilyl)but-1-en-3-yn-2-yl]-10*H*-phenothiazine

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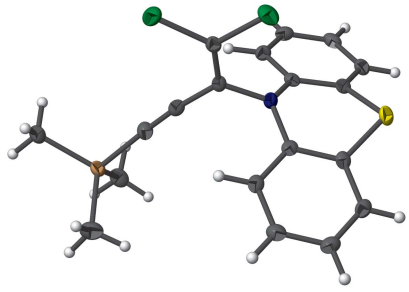
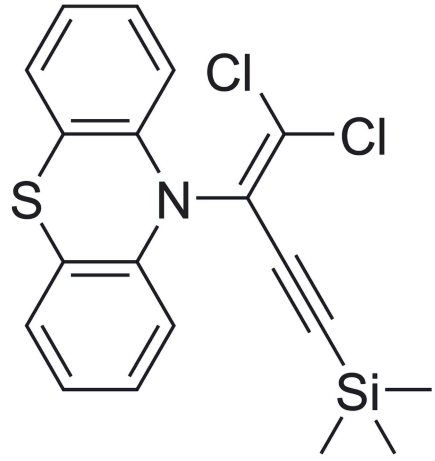
The title compound, $C_{19}H_{17}Cl_2NSSi$, is an enamine derivative, in which the N atom adopts a shallow trigonal–pyramidal geometry [displacement from the plane of its attached C atoms = 0.1383 (18) Å]. The dihedral angle between the plane through the three amino carbon atoms and the vinyl group is 89.47 (7)°. The phenothiazine unit has a butterfly structure and the central six-membered ring adopts a boat conformation. The fold angle between the benzene rings is 28.52 (7)°. The crystal structure features weak C*sp*^{3}—H···Cl hydrogen bonds, H···S contacts and π–π stacking interactions between phenothiazine units.

3D view



Chemical scheme



Structure description

Enamine was coined as a nitrogen analogue of enol (Kuehne, 1970; Valentine & Scott, 1978; Hickmott, 1982; Whitesell & Whitesell, 1983). An enamine unit is incorporated by many important natural products (Yet, 2003), and halogen-substituted enamines play a significant role as building blocks in organic synthesis (Geary & Hultin, 2009; Mansfield *et al.*, 2015).

The N1/C1/C12/C13 amino group has a shallow trigonal–pyramidal geometry in which the nitrogen atom is displaced upwards from the C1/C12/C13 plane by 0.1383 (18) Å (Fig. 1). The dihedral angle between this plane and the vinyl group (N1/C13/C14/C15/Cl1/Cl2; r.m.s. deviation = 0.0185 Å) is 89.45 (2)°, indicating no conjugation between them. When a vinyl group at an N-position carries an electron-withdrawing substituent or a small geminal substituent, the planes have a small dihedral angle and good conjugation. (Lebedev *et al.*, 2002; Okuno & Iwahashi, 2013; Garg & Ling, 2015). However, the title compound has a twisted form because of the bulky eneyne group. The phenothiazine unit has a butterfly structure and the central six-membered ring adopts a boat conformation. The fold angle between the C1–C6 and C7–C12 rings is 28.52 (7)°. The angle is similar to

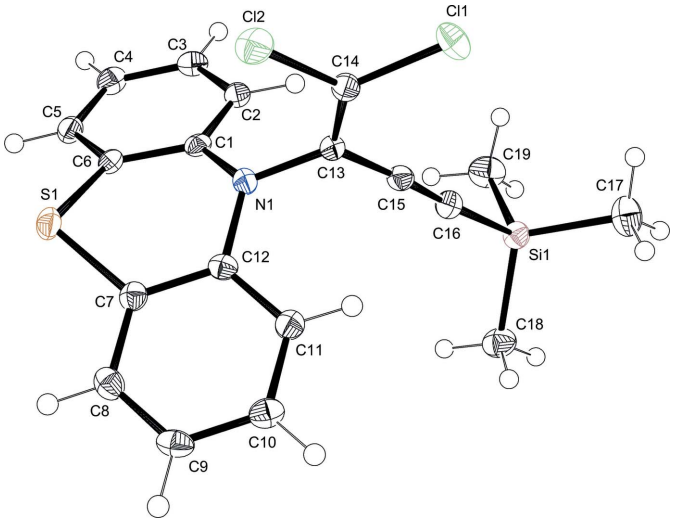


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level and H atoms are shown as small spheres.

those in other reported 10-vinyl-10*H*-phenothiazines (Ehmann *et al.*, 1994; Muller *et al.*, 2002; Umezono & Okuno, 2015).

The crystal structure (Fig. 2) features weak Csp^3—H···Cl hydrogen bonds (Table 1), H···S contacts [H5···S1^{iii} = 2.99 Å; symmetry code: (iii) $-x+2, -y, -z+1$] and π–π stacking interactions between the phenothiazine units [atoms C7–C12; $Cg\cdots Cg(-x+2, -y, -z)$ = 3.8002 (11) Å].

Synthesis and crystallization

Tetrakis(triphenylphosphine)palladium(0) (0.058 g, 0.050 mmol) was added to a solution of 10-(1,2,2-trichlorovinyl)-10*H*-phenothiazine (0.33 g, 1.0 mmol) (Okuno *et al.*, 2006) in toluene (10 ml) under an argon atmosphere. The solution was stirred at room temperature for 20 min, and copper(I) iodide (0.0095 g, 0.050 mmol), trimethylsilylacetylene (0.14 ml, 1.0 mmol) and diethylamine (0.15 ml, 1.5 mmol) were added to the solution. It was stirred at 313 K for 10 h, and then poured into 5% ammonium hydroxide. The organic layer was washed with water and dried over anhydrous sodium sulfate. After removal of sodium sulfate, it was concentrated by a rotary evaporator. The residue was purified by column chromatography on a silica gel with hexane as an eluent to give the title compound (0.19 g, 49%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.23 (*s*, 9H); 6.89–6.93 (*m*, 4H); 7.02–7.09 (*m*, 4H). Single crystals of sufficient quality for X-ray crystallographic analysis were prepared by recrystallization from a dichloromethane solution.

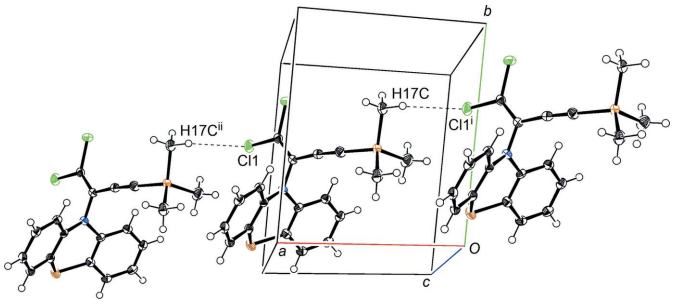


Figure 2
A view of the intermolecular interactions in the title compound [symmetry codes:(i) $x-1, y, z-1$; (ii) $x+1, y-1, z+1$].

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

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17C···Cl1^{i}	0.98	2.80	3.685 (3)	150

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{17}Cl_2NSSi$
M_r	390.40
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	93
a, b, c (Å)	10.073 (3), 10.370 (3), 10.547 (3)
α, β, γ (°)	105.029 (2), 115.480 (5), 90.3532 (15)
V (Å^3)	951.8 (4)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.51
Crystal size (mm)	0.10 × 0.10 × 0.01
Data collection	
Diffractometer	Rigaku Saturn724+
Absorption correction	Numerical (*NUMABS*; Rigaku, 1999)
T_{min}, T_{max}	0.961, 0.995
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	6593, 3294, 2802
R_{int}	0.019
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.075, 1.05
No. of reflections	3294
No. of parameters	220
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.22

Computer programs: *CrystalClear* (Rigaku, 2008), *SIR92* (Altomare *et al.*, 1994), *SHELXL2013* (Gruene *et al.*, 2014), *OPTEP-3 for Windows* (Farrugia, 2012) and *CrystalStructure* (Rigaku, 2014).

Refinement

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

Funding information

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full crystallographic data

IUCrData (2018). **3**, x180232 [https://doi.org/10.1107/S2414314618002328]

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Crystal data

$C_{19}H_{17}Cl_2NSSi$
M_r = 390.40
Triclinic, $P\overline{1}$
a = 10.073 (3) Å
b = 10.370 (3) Å
c = 10.547 (3) Å
α = 105.029 (2)°
β = 115.480 (5)°
γ = 90.3532 (15)°
V = 951.8 (4) Å^3
Z = 2
$F(000)$ = 404.00
D_x = 1.362 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 3280 reflections
θ = 2.1–31.1°
μ = 0.51 mm^{-1}
T = 93 K
Chip, colorless
0.10 × 0.10 × 0.01 mm

Data collection

Rigaku Saturn724+ diffractometer
Detector resolution: 7.111 pixels mm^{-1}
ω scans
Absorption correction: numerical (*NUMABS*; Rigaku, 1999)
T_{min} = 0.961, T_{max} = 0.995
6593 measured reflections
3294 independent reflections
2802 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.019
θ_{max} = 25.0°, θ_{min} = 2.1°
h = −10→11
k = −12→12
l = −12→12

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.075
S = 1.05
3294 reflections
220 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
$w = 1/[\sigma^2(F_o^2) + (0.0311P)^2 + 0.618P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY
Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).
The C-bound H atoms were placed at ideal positions and were refined as riding on their parent C atoms. U_{iso}(H) values of the H atoms were set at 1.2U_{eq}(parent atom for C_{sp2}) and 1.5 U_{eq}(parent atom for C_{sp3}).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.15825 (6)	0.49602 (5)	0.45814 (5)	0.02756 (14)
Cl2	0.99925 (6)	0.66282 (5)	0.27723 (6)	0.02713 (14)
S1	1.11156 (6)	0.03876 (5)	0.33623 (5)	0.02274 (13)
Si1	0.55882 (6)	0.36903 (6)	−0.24744 (6)	0.01966 (14)
N1	0.97946 (17)	0.26504 (16)	0.21053 (17)	0.0167 (3)
C1	0.8870 (2)	0.19488 (18)	0.24819 (19)	0.0162 (4)
C2	0.7498 (2)	0.23375 (19)	0.2328 (2)	0.0190 (4)
C3	0.6616 (2)	0.1646 (2)	0.2722 (2)	0.0213 (4)
C4	0.7072 (2)	0.0548 (2)	0.3235 (2)	0.0228 (4)
C5	0.8424 (2)	0.0142 (2)	0.3367 (2)	0.0208 (4)
C6	0.9339 (2)	0.08561 (19)	0.3031 (2)	0.0179 (4)
C7	1.1366 (2)	0.08824 (19)	0.1992 (2)	0.0180 (4)
C8	1.2287 (2)	0.0224 (2)	0.1445 (2)	0.0215 (4)
C9	1.2651 (2)	0.0688 (2)	0.0496 (2)	0.0217 (4)
C10	1.2059 (2)	0.1788 (2)	0.0071 (2)	0.0215 (4)
C11	1.1088 (2)	0.24270 (19)	0.0571 (2)	0.0191 (4)
C12	1.0741 (2)	0.19844 (19)	0.1545 (2)	0.0163 (4)
C13	0.9441 (2)	0.39215 (19)	0.1853 (2)	0.0162 (4)
C14	1.0224 (2)	0.50325 (19)	0.2928 (2)	0.0177 (4)
C15	0.8274 (2)	0.39420 (19)	0.0461 (2)	0.0187 (4)
C16	0.7258 (2)	0.3840 (2)	−0.0724 (2)	0.0216 (4)
C17	0.5561 (2)	0.5327 (2)	−0.2888 (3)	0.0301 (5)
C18	0.3951 (3)	0.3323 (2)	−0.2177 (3)	0.0329 (5)
C19	0.5650 (2)	0.2299 (2)	−0.3960 (2)	0.0282 (5)
H2	0.7164	0.30766	0.19539	0.0228*
H3	0.56949	0.19308	0.26379	0.0256*
H4	0.64632	0.00742	0.34948	0.0273*
H5	0.87268	−0.06295	0.36892	0.0250*
H8	1.26701	−0.05481	0.17204	0.0258*
H9	1.3304	0.02514	0.01435	0.0260*
H10	1.23141	0.21134	−0.05689	0.0257*
H11	1.06626	0.31662	0.02465	0.0229*
H17A	0.64503	0.55237	−0.3001	0.0361*
H17B	0.55442	0.60431	−0.20813	0.0361*
H17C	0.46744	0.52785	−0.37997	0.0361*
H18A	0.38876	0.40995	−0.14523	0.0395*
H18B	0.40566	0.25301	−0.18174	0.0395*
H18C	0.30463	0.31468	−0.31061	0.0395*
H19A	0.55969	0.14409	−0.37458	0.0339*
H19B	0.65794	0.24554	−0.402	0.0339*
H19C	0.48075	0.22678	−0.48976	0.0339*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0214 (3)	0.0318 (3)	0.0189 (3)	0.0017 (2)	0.0021 (2)	0.0029 (2)
Cl2	0.0284 (3)	0.0160 (3)	0.0364 (3)	0.0035 (2)	0.0145 (2)	0.0066 (2)
S1	0.0221 (3)	0.0290 (3)	0.0209 (3)	0.0094 (2)	0.0091 (2)	0.0140 (2)
Si1	0.0163 (3)	0.0226 (3)	0.0180 (3)	0.0032 (2)	0.0053 (2)	0.0067 (2)
N1	0.0177 (8)	0.0165 (8)	0.0179 (8)	0.0047 (6)	0.0086 (7)	0.0068 (7)
C1	0.0189 (10)	0.0154 (9)	0.0106 (9)	−0.0008 (7)	0.0054 (8)	0.0002 (8)
C2	0.0221 (10)	0.0174 (10)	0.0155 (10)	0.0030 (8)	0.0072 (8)	0.0036 (8)
C3	0.0198 (10)	0.0226 (11)	0.0196 (10)	0.0006 (8)	0.0095 (9)	0.0018 (8)
C4	0.0254 (11)	0.0217 (11)	0.0210 (10)	−0.0023 (8)	0.0111 (9)	0.0047 (9)
C5	0.0268 (11)	0.0186 (10)	0.0174 (10)	0.0024 (8)	0.0096 (9)	0.0062 (8)
C6	0.0203 (10)	0.0198 (10)	0.0112 (9)	0.0040 (8)	0.0052 (8)	0.0041 (8)
C7	0.0157 (10)	0.0195 (10)	0.0149 (9)	0.0009 (8)	0.0038 (8)	0.0041 (8)
C8	0.0178 (10)	0.0201 (10)	0.0208 (10)	0.0035 (8)	0.0045 (9)	0.0042 (8)
C9	0.0160 (10)	0.0237 (11)	0.0195 (10)	0.0020 (8)	0.0072 (8)	−0.0016 (9)
C10	0.0205 (10)	0.0225 (11)	0.0211 (10)	−0.0016 (8)	0.0110 (9)	0.0031 (9)
C11	0.0201 (10)	0.0180 (10)	0.0178 (10)	0.0007 (8)	0.0077 (8)	0.0043 (8)
C12	0.0136 (9)	0.0164 (10)	0.0136 (9)	−0.0004 (7)	0.0037 (8)	−0.0001 (8)
C13	0.0177 (10)	0.0167 (10)	0.0159 (9)	0.0041 (8)	0.0085 (8)	0.0056 (8)
C14	0.0162 (10)	0.0198 (10)	0.0192 (10)	0.0043 (8)	0.0091 (8)	0.0067 (8)
C15	0.0221 (11)	0.0172 (10)	0.0204 (10)	0.0035 (8)	0.0126 (9)	0.0055 (8)
C16	0.0231 (11)	0.0221 (11)	0.0197 (11)	0.0051 (8)	0.0091 (9)	0.0071 (9)
C17	0.0214 (11)	0.0300 (12)	0.0299 (12)	0.0020 (9)	0.0013 (10)	0.0125 (10)
C18	0.0273 (12)	0.0344 (13)	0.0369 (13)	−0.0001 (10)	0.0172 (11)	0.0053 (11)
C19	0.0256 (11)	0.0341 (12)	0.0201 (11)	0.0037 (9)	0.0077 (9)	0.0047 (9)

Geometric parameters (Å, º)

Cl1—C14	1.7128 (19)	C11—C12	1.393 (4)
Cl2—C14	1.713 (2)	C13—C14	1.333 (2)
S1—C6	1.766 (2)	C13—C15	1.438 (3)
S1—C7	1.765 (3)	C15—C16	1.204 (3)
Si1—C16	1.8545 (19)	C2—H2	0.950
Si1—C17	1.856 (3)	C3—H3	0.950
Si1—C18	1.860 (3)	C4—H4	0.950
Si1—C19	1.858 (2)	C5—H5	0.950
N1—C1	1.420 (3)	C8—H8	0.950
N1—C12	1.420 (3)	C9—H9	0.950
N1—C13	1.429 (3)	C10—H10	0.950
C1—C2	1.395 (3)	C11—H11	0.950
C1—C6	1.398 (3)	C17—H17A	0.980
C2—C3	1.393 (4)	C17—H17B	0.980
C3—C4	1.383 (3)	C17—H17C	0.980
C4—C5	1.388 (3)	C18—H18A	0.980
C5—C6	1.390 (4)	C18—H18B	0.980
C7—C8	1.386 (3)	C18—H18C	0.980

C7—C12	1.399 (3)	C19—H19A	0.980
C8—C9	1.390 (4)	C19—H19B	0.980
C9—C10	1.379 (3)	C19—H19C	0.980
C10—C11	1.394 (3)		
Cl1···N1	2.9081 (14)	C15···H11^{iv}	3.5367
Cl2···C15	3.0800 (18)	C15···H18A^{vii}	3.2968
S1···N1	3.0280 (19)	C16···H8^{iii}	3.3125
N1···C16	3.513 (3)	C16···H11^{iv}	3.5327
C1···C4	2.798 (4)	C16···H18A^{vii}	3.3061
C1···C7	2.945 (3)	C17···H2^{vii}	3.5752
C1···C14	3.305 (3)	C17···H3^{vii}	3.1143
C1···C15	3.221 (3)	C17···H17C^{xii}	3.2869
C2···C5	2.774 (3)	C18···H4^{x}	3.3855
C2···C13	2.830 (3)	C18···H5^{x}	3.3938
C2···C15	3.204 (4)	C18···H10^{viii}	3.2643
C3···C6	2.775 (3)	C19···H3^{xiii}	3.5287
C6···C12	2.942 (4)	C19···H4^{xiii}	3.4500
C7···C10	2.769 (4)	C19···H4^{x}	3.5059
C8···C11	2.774 (3)	C19···H8^{iii}	3.2502
C9···C12	2.797 (3)	H2···Cl1^{i}	3.3516
C11···C13	2.804 (3)	H2···C17^{vii}	3.5752
C11···C14	3.556 (3)	H2···H9^{iii}	3.4857
C11···C15	3.223 (3)	H2···H17B^{vii}	2.9284
C12···C14	3.267 (3)	H2···H17C^{vii}	3.3981
C12···C15	3.229 (3)	H2···H18A^{vii}	3.2152
C14···C16	3.588 (2)	H3···C8^{viii}	3.3993
Cl1···C2^{i}	3.4595 (19)	H3···C9^{viii}	2.9402
S1···C5^{ii}	3.468 (3)	H3···C10^{viii}	3.4671
C1···C9^{iii}	3.324 (2)	H3···C17^{vii}	3.1143
C2···Cl1^{i}	3.4595 (19)	H3···C19^{ix}	3.5287
C5···S1^{ii}	3.468 (3)	H3···H8^{viii}	3.5923
C5···C9^{iii}	3.590 (3)	H3···H9^{viii}	2.8063
C5···C10^{iii}	3.478 (3)	H3···H17A^{vii}	3.4702
C6···C9^{iii}	3.298 (2)	H3···H17B^{vii}	2.5216
C6···C10^{iii}	3.397 (2)	H3···H17C^{vii}	2.9294
C8···C12^{iii}	3.519 (2)	H3···H19B^{ix}	3.1325
C9···C1^{iii}	3.324 (2)	H3···H19C^{ix}	3.0348
C9···C5^{iii}	3.590 (3)	H4···S1^{ii}	3.3238
C9···C6^{iii}	3.298 (2)	H4···C18^{x}	3.3855
C10···C5^{iii}	3.478 (3)	H4···C19^{ix}	3.4500
C10···C6^{iii}	3.397 (2)	H4···C19^{x}	3.5059
C10···C17^{iv}	3.564 (3)	H4···H8^{viii}	3.4217
C11···C17^{iv}	3.556 (3)	H4···H18B^{x}	2.7213
C12···C8^{iii}	3.519 (2)	H4···H18C^{x}	3.3247
C17···C10^{iv}	3.564 (3)	H4···H19A^{ix}	3.3618
C17···C11^{iv}	3.556 (3)	H4···H19A^{x}	2.7373
S1···H5	2.8093	H4···H19B^{ix}	3.0590

S1···H8	2.8058	H4···H19C^{ix}	3.3631
N1···H2	2.6323	H5···Cl2^{xiv}	3.2136
N1···H11	2.6281	H5···S1^{ii}	2.9882
C1···H3	3.2723	H5···C5^{ii}	3.1037
C1···H5	3.2726	H5···C6^{ii}	3.2323
C2···H4	3.2679	H5···C10^{iii}	3.5521
C3···H5	3.2515	H5···C18^{x}	3.3938
C4···H2	3.2643	H5···H5^{ii}	2.8131
C5···H3	3.2522	H5···H10^{iii}	2.9467
C6···H2	3.2667	H5···H18B^{x}	2.9655
C6···H4	3.2692	H5···H18C^{x}	2.9236
C7···H9	3.2659	H8···C15^{iii}	3.5303
C7···H11	3.2648	H8···C16^{iii}	3.3125
C8···H10	3.2498	H8···C19^{iii}	3.2502
C9···H11	3.2628	H8···H3^{xi}	3.5923
C10···H8	3.2490	H8···H4^{xi}	3.4217
C11···H9	3.2672	H8···H19A^{iii}	2.5110
C12···H8	3.2729	H8···H19B^{iii}	3.3608
C12···H10	3.2694	H9···C1^{iii}	3.0188
C13···H2	2.5044	H9···C2^{iii}	3.0313
C13···H11	2.4732	H9···C3^{xi}	3.2731
C14···H2	3.2846	H9···C3^{iii}	3.1843
C14···H11	3.1918	H9···C4^{iii}	3.2911
C15···H2	2.6014	H9···C5^{iii}	3.2509
C15···H11	2.6242	H9···C6^{iii}	3.1489
C16···H2	3.1624	H9···H2^{iii}	3.4857
C16···H11	3.2675	H9···H3^{xi}	2.8063
C16···H17A	3.1608	H9···H9^{xv}	3.5871
C16···H17B	3.1414	H10···Cl2^{iv}	3.0768
C16···H18A	3.1723	H10···C5^{iii}	3.0400
C16···H18B	3.0836	H10···C6^{iii}	3.3269
C16···H19A	3.2246	H10···C18^{xi}	3.2643
C16···H19B	3.1577	H10···H5^{iii}	2.9467
C17···H18A	3.1503	H10···H17A^{iv}	3.5883
C17···H18C	3.2772	H10···H17B^{iv}	2.8481
C17···H19B	3.2548	H10···H18A^{xi}	3.1381
C17···H19C	3.1989	H10···H18B^{xi}	2.6974
C18···H17B	3.1933	H10···H18C^{xi}	3.4683
C18···H17C	3.2287	H11···Cl2^{iv}	3.0274
C18···H19A	3.1655	H11···C15^{iv}	3.5367
C18···H19C	3.2690	H11···C16^{iv}	3.5327
C19···H17A	3.2195	H11···H17A^{iv}	3.0624
C19···H17C	3.2327	H11···H17B^{iv}	3.4340
C19···H18B	3.2538	H17A···Cl1^{iv}	3.0622
C19···H18C	3.1804	H17A···C10^{iv}	3.3263
H2···H3	2.3374	H17A···C11^{iv}	2.9792
H3···H4	2.3327	H17A···C12^{iv}	3.3396
H4···H5	2.3386	H17A···C14^{iv}	3.3741

H8···H9	2.3417	H17A···H3^{vii}	3.4702
H9···H10	2.3278	H17A···H10^{iv}	3.5883
H10···H11	2.3378	H17A···H11^{iv}	3.0624
H17A···H19B	3.1062	H17A···H17C^{xii}	2.9335
H17A···H19C	3.4235	H17A···H19C^{xii}	3.4663
H17B···H18A	2.9819	H17B···C2^{vii}	3.4469
H17B···H18C	3.5218	H17B···C3^{vii}	3.2519
H17C···H18A	3.3910	H17B···C9^{iv}	3.4581
H17C···H18C	3.1524	H17B···C10^{iv}	2.9052
H17C···H19B	3.5224	H17B···C11^{iv}	3.2457
H17C···H19C	3.0611	H17B···H2^{vii}	2.9284
H18B···H19A	3.0603	H17B···H3^{vii}	2.5216
H18B···H19C	3.5860	H17B···H10^{iv}	2.8481
H18C···H19A	3.3337	H17B···H11^{iv}	3.4340
H18C···H19C	3.0918	H17B···H18A^{vii}	3.5625
Cl1···H2^{i}	3.3516	H17C···Cl1^{xvi}	2.8007
Cl1···H17A^{iv}	3.0622	H17C···C3^{vii}	3.5492
Cl1···H17C^{v}	2.8007	H17C···C17^{xii}	3.2869
Cl1···H18C^{v}	3.3133	H17C···H2^{vii}	3.3981
Cl1···H19B^{iv}	3.5590	H17C···H3^{vii}	2.9294
Cl2···H5^{vi}	3.2136	H17C···H17A^{xii}	2.9335
Cl2···H10^{iv}	3.0768	H17C···H17C^{xii}	2.8018
Cl2···H11^{iv}	3.0274	H17C···H19B^{xii}	3.5702
Cl2···H18A^{vii}	3.5384	H17C···H19C^{xii}	3.3239
Cl2···H18C^{vii}	3.2313	H18A···Cl2^{vii}	3.5384
Cl2···H19B^{iv}	3.1559	H18A···C15^{vii}	3.2968
S1···H4^{ii}	3.3238	H18A···C16^{vii}	3.3061
S1···H5^{ii}	2.9882	H18A···H2^{vii}	3.2152
C1···H9^{iii}	3.0188	H18A···H10^{viii}	3.1381
C2···H9^{iii}	3.0313	H18A···H17B^{vii}	3.5625
C2···H17B^{vii}	3.4469	H18A···H18A^{vii}	2.9950
C3···H9^{viii}	3.2731	H18B···C4^{x}	3.1195
C3···H9^{iii}	3.1843	H18B···C5^{x}	3.2626
C3···H17B^{vii}	3.2519	H18B···C10^{viii}	3.5828
C3···H17C^{vii}	3.5492	H18B···H4^{x}	2.7213
C3···H19B^{ix}	3.3358	H18B···H5^{x}	2.9655
C4···H9^{iii}	3.2911	H18B···H10^{viii}	2.6974
C4···H18B^{x}	3.1195	H18C···Cl1^{xvi}	3.3133
C4···H19B^{ix}	3.2894	H18C···Cl2^{vii}	3.2313
C5···H5^{ii}	3.1037	H18C···H4^{x}	3.3247
C5···H9^{iii}	3.2509	H18C···H5^{x}	2.9236
C5···H10^{iii}	3.0400	H18C···H10^{viii}	3.4683
C5···H18B^{x}	3.2626	H19A···C8^{iii}	3.3438
C6···H5^{ii}	3.2323	H19A···H4^{xiii}	3.3618
C6···H9^{iii}	3.1489	H19A···H4^{x}	2.7373
C6···H10^{iii}	3.3269	H19A···H8^{iii}	2.5110
C7···H19C^{v}	3.5429	H19A···H19A^{xvii}	3.2395
C8···H3^{xi}	3.3993	H19B···Cl1^{iv}	3.5590

C8···H19A^{iii}	3.3438	H19B···Cl2^{iv}	3.1559
C9···H3^{xi}	2.9402	H19B···C3^{xiii}	3.3358
C9···H17B^{iv}	3.4581	H19B···C4^{xiii}	3.2894
C10···H3^{xi}	3.4671	H19B···H3^{xiii}	3.1325
C10···H5^{iii}	3.5521	H19B···H4^{xiii}	3.0590
C10···H17A^{iv}	3.3263	H19B···H8^{iii}	3.3608
C10···H17B^{iv}	2.9052	H19B···H17C^{xii}	3.5702
C10···H18B^{xi}	3.5828	H19C···C7^{xvi}	3.5429
C11···H17A^{iv}	2.9792	H19C···H3^{xiii}	3.0348
C11···H17B^{iv}	3.2457	H19C···H4^{xiii}	3.3631
C12···H17A^{iv}	3.3396	H19C···H17A^{xii}	3.4663
C14···H17A^{iv}	3.3741	H19C···H17C^{xii}	3.3239
C15···H8^{iii}	3.5303		

C6—S1—C7	99.94 (10)	C13—C15—C16	174.2 (2)
C16—Si1—C17	107.98 (9)	Si1—C16—C15	175.2 (2)
C16—Si1—C18	106.78 (12)	C1—C2—H2	119.879
C16—Si1—C19	109.66 (10)	C3—C2—H2	119.882
C17—Si1—C18	110.46 (12)	C2—C3—H3	119.748
C17—Si1—C19	111.21 (12)	C4—C3—H3	119.747
C18—Si1—C19	110.61 (11)	C3—C4—H4	120.232
C1—N1—C12	121.74 (17)	C5—C4—H4	120.241
C1—N1—C13	118.20 (18)	C4—C5—H5	119.771
C12—N1—C13	117.3 (2)	C6—C5—H5	119.790
N1—C1—C2	121.17 (18)	C7—C8—H8	119.843
N1—C1—C6	119.80 (19)	C9—C8—H8	119.842
C2—C1—C6	119.0 (2)	C8—C9—H9	120.260
C1—C2—C3	120.2 (2)	C10—C9—H9	120.261
C2—C3—C4	120.5 (2)	C9—C10—H10	119.661
C3—C4—C5	119.5 (2)	C11—C10—H10	119.661
C4—C5—C6	120.4 (2)	C10—C11—H11	119.928
S1—C6—C1	121.02 (18)	C12—C11—H11	119.917
S1—C6—C5	118.77 (16)	Si1—C17—H17A	109.475
C1—C6—C5	120.2 (2)	Si1—C17—H17B	109.469
S1—C7—C8	118.71 (16)	Si1—C17—H17C	109.467
S1—C7—C12	120.68 (18)	H17A—C17—H17B	109.471
C8—C7—C12	120.4 (2)	H17A—C17—H17C	109.471
C7—C8—C9	120.3 (2)	H17B—C17—H17C	109.474
C8—C9—C10	119.5 (2)	Si1—C18—H18A	109.471
C9—C10—C11	120.7 (2)	Si1—C18—H18B	109.477
C10—C11—C12	120.2 (2)	Si1—C18—H18C	109.469
N1—C12—C7	120.1 (2)	H18A—C18—H18B	109.470
N1—C12—C11	121.01 (19)	H18A—C18—H18C	109.468
C7—C12—C11	118.9 (2)	H18B—C18—H18C	109.473
N1—C13—C14	117.78 (16)	Si1—C19—H19A	109.468
N1—C13—C15	118.82 (14)	Si1—C19—H19B	109.470
C14—C13—C15	123.40 (19)	Si1—C19—H19C	109.467
Cl1—C14—Cl2	114.66 (9)	H19A—C19—H19B	109.479

Cl1—C14—C13	121.79 (17)	H19A—C19—H19C	109.469
Cl2—C14—C13	123.53 (16)	H19B—C19—H19C	109.474
C6—S1—C7—C8	−153.30 (11)	C6—C1—C2—C3	0.2 (2)
C6—S1—C7—C12	31.54 (13)	C1—C2—C3—C4	−1.6 (2)
C7—S1—C6—C1	−30.81 (13)	C2—C3—C4—C5	0.5 (2)
C7—S1—C6—C5	151.08 (12)	C3—C4—C5—C6	2.0 (3)
C1—N1—C12—C7	−31.93 (19)	C4—C5—C6—S1	174.73 (14)
C1—N1—C12—C11	149.39 (14)	C4—C5—C6—C1	−3.4 (2)
C12—N1—C1—C2	−147.89 (14)	S1—C7—C8—C9	−172.33 (10)
C12—N1—C1—C6	32.7 (2)	S1—C7—C12—N1	−5.17 (19)
C1—N1—C13—C14	101.0 (2)	S1—C7—C12—C11	173.54 (9)
C1—N1—C13—C15	−79.4 (2)	C8—C7—C12—N1	179.75 (12)
C13—N1—C1—C2	12.6 (2)	C8—C7—C12—C11	−1.5 (2)
C13—N1—C1—C6	−166.74 (12)	C12—C7—C8—C9	2.8 (2)
C12—N1—C13—C14	−97.6 (2)	C7—C8—C9—C10	−1.7 (2)
C12—N1—C13—C15	82.0 (2)	C8—C9—C10—C11	−0.7 (2)
C13—N1—C12—C7	167.38 (12)	C9—C10—C11—C12	2.0 (2)
C13—N1—C12—C11	−11.30 (19)	C10—C11—C12—N1	177.85 (13)
N1—C1—C2—C3	−179.17 (13)	C10—C11—C12—C7	−0.8 (2)
N1—C1—C6—S1	3.6 (2)	N1—C13—C14—Cl1	−1.6 (3)
N1—C1—C6—C5	−178.35 (13)	N1—C13—C14—Cl2	177.13 (18)
C2—C1—C6—S1	−175.80 (12)	C15—C13—C14—Cl1	178.8 (2)
C2—C1—C6—C5	2.3 (2)	C15—C13—C14—Cl2	−2.5 (4)

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) −*x*+2, −*y*, −*z*+1; (iii) −*x*+2, −*y*, −*z*; (iv) −*x*+2, −*y*+1, −*z*; (v) *x*+1, *y*, *z*+1; (vi) *x*, *y*+1, *z*; (vii) −*x*+1, −*y*+1, −*z*; (viii) *x*−1, *y*, *z*; (ix) *x*, *y*, *z*+1; (x) −*x*+1, −*y*, −*z*; (xi) *x*+1, *y*, *z*; (xii) −*x*+1, −*y*+1, −*z*−1; (xiii) *x*, *y*, *z*−1; (xiv) *x*, *y*−1, *z*; (xv) −*x*+3, −*y*, −*z*; (xvi) *x*−1, *y*, *z*−1; (xvii) −*x*+1, −*y*, −*z*−1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17*C*···Cl1^{xvi}	0.98	2.80	3.685 (3)	150

Symmetry code: (xvi) *x*−1, *y*, *z*−1.