

1-Benzyl-3-[(trimethylsilyl)methyl]-benzimidazolium chloride monohydrate

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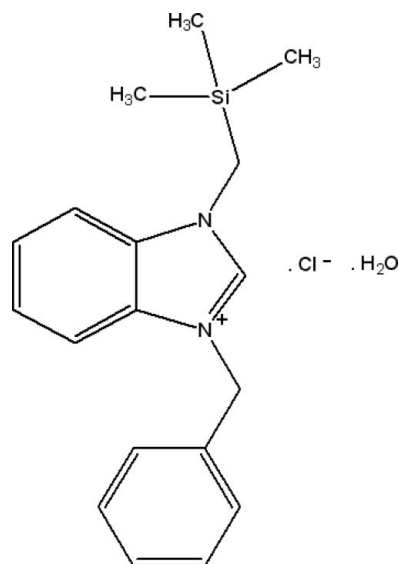
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.049; wR factor = 0.135; data-to-parameter ratio = 18.9.

The title compound, $\text{C}_{18}\text{H}_{23}\text{N}_2\text{Si}^+\cdot\text{Cl}^-\cdot\text{H}_2\text{O}$, was synthesized from 1-[(trimethylsilyl)methyl]benzimidazole and benzyl chloride in dimethylformamide. The benzimidazole ring system is approximately planar, with a maximum deviation of 0.022 (2) Å, and makes an angle of 74.80 (12)° with the phenyl ring. The crystal packing is stabilized by $\text{O}-\text{H}\cdots\text{Cl}$, $\text{C}-\text{H}\cdots\text{Cl}$, $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\pi$ interactions between symmetry-related molecules together with $\pi-\pi$ stacking interactions between the imidazolium and benzene rings [centroid-centroid distance = 3.5690 (15) Å] and between the benzene rings [centroid-centroid distance = 3.7223 (14) Å].

Related literature

For general background to benzimidazole compounds and for the biological activity of related structures, see: Galal *et al.* (2009); Huang *et al.* (2006); Küçükbay & Durmaz (1997); Küçükbay *et al.* (1995, 2003, 2004, 2010); Lukevics *et al.* (2001); Singh & Lown (2000); Tavman *et al.* (2005); Turner & Denny (1996); Williams *et al.* (2002); Yılmaz & Küçükbay (2009); Çetinkaya *et al.* (1996). For similar structures, see: Akkurt *et al.* (2008, 2010).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{23}\text{N}_2\text{Si}^+\cdot\text{Cl}^-\cdot\text{H}_2\text{O}$

$M_r = 348.94$

Triclinic, $P\bar{1}$

$a = 9.3592$ (7) Å

$b = 10.9500$ (9) Å

$c = 11.0522$ (8) Å

$\alpha = 117.594$ (6)°

$\beta = 103.295$ (6)°

$\gamma = 92.094$ (6)°

$V = 963.39$ (15) Å³

$Z = 2$

Mo $K\alpha$ radiation

$\mu = 0.27$ mm⁻¹

$T = 296$ K

$0.57 \times 0.50 \times 0.36$ mm

Data collection

Stoe IPDS 2 diffractometer

Absorption correction: integration

(*X-RED32*; Stoe & Cie, 2002)

$T_{\min} = 0.859$, $T_{\max} = 0.909$

12149 measured reflections

3987 independent reflections

3241 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.135$

$S = 1.07$

3987 reflections

211 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.32$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.32$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg3 is the centroid of the C9–C14 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O1–H1A \cdots Cl1	0.86	2.45	3.257 (2)	157
O1–H1B \cdots Cl1 ⁱ	0.85	2.45	3.250 (3)	158
C7–H7 \cdots O1	0.93	2.51	3.170 (3)	128
C8–H8A \cdots Cl1	0.97	2.81	3.703 (2)	153
C3–H3 \cdots Cg3 ⁱⁱ	0.93	2.69	3.526 (2)	151

Symmetry codes: (i) $-x + 2, -y + 1, -z + 2$; (ii) $x - 1, y, z$.

Data collection: *X-Area* (Stoe & Cie, 2002); cell refinement: *X-Area*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-III* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2582).

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supplementary materials

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1-Benzyl-3-[(trimethylsilyl)methyl]benzimidazolium chloride monohydrate

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Comment

Although there are different antibacterial and antifungal drugs used in the treatment of bacterial and fungal infections, some of them have undesirable side effects. In addition, some of them become less effective due to the development of resistance to these drugs (Williams *et al.*, 2002). Therefore, many clinically effective antibacterial and antifungal drugs have become less effective due to the development of resistance to these drugs. Since, benzimidazole compounds have been found to have a broad range of pharmacological activity, many research groups as well as our group have been interested in these type of heterocyclic compounds (Singh *et al.*, 2000; Huang *et al.* 2006; Turner & Denny, 1996; Lukevics *et al.*, 2001; Galal *et al.* 2009; Çetinkaya *et al.*, 1996; Küçükbay *et al.*, 1995, 1997, 2003, 2004, 2010; Yılmaz & Küçükbay, 2009; Tavman *et al.*, 2005). In recent years, considerable attention has been given to the synthesis of alkylsilyl substituted benzimidazole derivatives because of their properties in cancer therapy. For example, 1-(3-trimethylsilylpropyl)benzimidazole inhibits carcinoma S-180 tumour growth in dose 1 mg.kg⁻¹ by 62% (on ICR mice) (Lukevics *et al.*, 2001). These properties of silylsubstituted benzimidazole compounds, triggered us to synthesis novel trimethylsilyl substituted benzimidazole compounds. The objectives of this study were to synthesize and elucidate the crystal structure of the title compound, 1-benzyl-3-trimethylsilylmethylbenzimidazolium chloride monohydrate, (I).

In the title molecule, (Fig. 1), the benzimidazole ring system (N1/N2/C1–C7) is approximately planar, with maximum deviations of -0.022 (2) Å for C6, -0.018 (2) for C1 and 0.015 (2) for C7. The benzimidazole (N1/N2/C1–C7) and phenyl (C9–C14) systems make an angle of 74.80 (12)°. The values of the geometric parameters in (I) are comparable with those observed for other similar compounds (Akkurt *et al.*, 2008, 2010). The average value of the Si—C bond length is 1.854 (4) Å. The angles around the Si atoms with a distorted tetrahedral geometry rang from 105.86 (16)° to 111.81 (16)°.

The crystal packing of (I) is stabilized by O—H···Cl, C—H···Cl and C—H···π interactions between symmetry-related molecules (Fig. 2 and Table 1), together with π-π stacking interactions between imidazolium and benzene (Table 2).

Experimental

A mixture of 1-trimethylsilylmethylbenzimidazole (1.02 g, 5 mmol) and benzyl chloride (0.60 cm³, 5 mmol) in dimethylformamide (5 ml) was refluxed for 3 h. The mixture was then cooled and the volatiles were removed *in vacuo*. The residue was crystallized from a dimethylformamide/ethanol (1:1). White crystals of the title compound (1.36 g, 82%) were obtained, m.p. 425–426 K; $\nu_{(\text{CN})}$ = 1553 cm⁻¹. Anal. Found: C 61.64, H 7.19, N 7.93%. Calculated for C₁₈H₂₅ClN₂OSi: C 61.96, H 7.22, N 8.03%. ¹H NMR (δ, DMSO-d₆): 10.21 (s, 1H, NCHN), 8.11 - 7.59 (m, 4H, C₆H₄), 7.56–7.33 (m, 5H, C₆H₅), 5.86 (s, 2H, CH₂ benzyl), 4.30 (s, 2H, CH₂Si) and 0.14 [s, 9H, (CH₃)₃Si]. ¹³C NMR (δ, DMSO-d₆): 141.6 (NCHN), 134.6, 132.1, 130.8, 129.1, 128.8 and 128.3 (C₆H₄), 126.8, 126.5, 114.3 and 113.9 (C₆H₅), 49.8 (CH₂ benzyl), 38.1(CH₂Si) and -2.5 [(CH₃)₃Si].

Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic), 0.96 Å (methyl) and 0.97 Å (methylene) with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl})$. H atoms of water molecule were located in difference Fourier maps and included in the subsequent refinement using restraints (O—H = 0.83 (1)Å and H···H = 1.40 (2)Å) with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. In the last cycles of refinement, they were treated as riding on the O atoms.

Figures

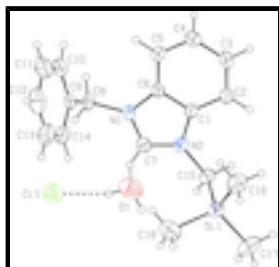


Fig. 1. View of the title molecule in the asymmetric unit, with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii and H bonds are shown as dashed lines.

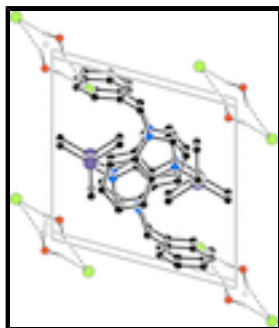


Fig. 2. View of the packing and hydrogen bonding interactions of (I) down the *b* axis. All hydrogen atoms not involved in hydrogen bonding have been omitted for clarity.

1-Benzyl-3-[(trimethylsilyl)methyl]benzimidazolium chloride monohydrate

Crystal data

$\text{C}_{18}\text{H}_{23}\text{N}_2\text{Si}^+\cdot\text{Cl}^-\cdot\text{H}_2\text{O}$

$M_r = 348.94$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 9.3592(7)$ Å

$b = 10.9500(9)$ Å

$c = 11.0522(8)$ Å

$\alpha = 117.594(6)^\circ$

$\beta = 103.295(6)^\circ$

$\gamma = 92.094(6)^\circ$

$V = 963.39(15)$ Å³

$Z = 2$

$F(000) = 372$

$D_x = 1.203$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 28124 reflections

$\theta = 2.1\text{--}28.0^\circ$

$\mu = 0.27$ mm⁻¹

$T = 296$ K

Prism, colourless

$0.57 \times 0.50 \times 0.36$ mm

Data collection

Stoe IPDS 2 diffractometer	3987 independent reflections
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus plane graphite	3241 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{\text{int}} = 0.029$
ω scans	$\theta_{\text{max}} = 26.5^\circ$, $\theta_{\text{min}} = 2.1^\circ$ $h = -11 \rightarrow 11$
Absorption correction: integration (<i>X-RED32</i> ; Stoe & Cie, 2002)	$k = -13 \rightarrow 12$
$T_{\text{min}} = 0.859$, $T_{\text{max}} = 0.909$	$l = -13 \rightarrow 13$
12149 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.049$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.135$	H-atom parameters constrained
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0637P)^2 + 0.2683P]$
3987 reflections	where $P = (F_o^2 + 2F_c^2)/3$
211 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.32 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.32 \text{ e } \text{\AA}^{-3}$

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.

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *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 R -factors based on ALL data will be even larger.

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	0.53328 (7)	0.20172 (7)	0.79168 (6)	0.05705 (19)
N1	0.72385 (17)	0.36741 (17)	0.52896 (17)	0.0466 (4)
N2	0.59349 (17)	0.36730 (17)	0.66907 (17)	0.0466 (4)

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C1	0.4923 (2)	0.33506 (19)	0.54087 (19)	0.0428 (4)
C2	0.3377 (2)	0.3101 (2)	0.4971 (2)	0.0521 (5)
H2	0.2816	0.3104	0.5566	0.063*
C3	0.2721 (2)	0.2847 (2)	0.3611 (2)	0.0587 (5)
H3	0.1688	0.2667	0.3276	0.070*
C4	0.3560 (2)	0.2853 (3)	0.2717 (2)	0.0592 (5)
H4	0.3071	0.2682	0.1806	0.071*
C5	0.5084 (2)	0.3104 (2)	0.3150 (2)	0.0532 (5)
H5	0.5641	0.3111	0.2555	0.064*
C6	0.57570 (19)	0.33479 (19)	0.4512 (2)	0.0432 (4)
C7	0.7293 (2)	0.3855 (2)	0.6574 (2)	0.0505 (5)
H7	0.8165	0.4079	0.7293	0.061*
C8	0.8534 (2)	0.3833 (2)	0.4794 (2)	0.0547 (5)
H8A	0.9413	0.4273	0.5602	0.066*
H8B	0.8371	0.4442	0.4377	0.066*
C9	0.8803 (2)	0.2461 (2)	0.3720 (2)	0.0510 (5)
C10	0.8520 (3)	0.2111 (3)	0.2308 (3)	0.0717 (7)
H10	0.8171	0.2741	0.2014	0.086*
C11	0.8748 (3)	0.0831 (4)	0.1329 (3)	0.0935 (10)
H11	0.8546	0.0600	0.0377	0.112*
C12	0.9272 (3)	-0.0100 (3)	0.1753 (4)	0.0947 (10)
H12	0.9404	-0.0970	0.1089	0.114*
C13	0.9600 (3)	0.0255 (3)	0.3158 (4)	0.0909 (10)
H13	0.9980	-0.0367	0.3451	0.109*
C14	0.9372 (3)	0.1527 (3)	0.4141 (3)	0.0700 (7)
H14	0.9602	0.1760	0.5095	0.084*
C15	0.5549 (3)	0.3754 (2)	0.7947 (2)	0.0549 (5)
H15A	0.4625	0.4122	0.8003	0.066*
H15B	0.6320	0.4406	0.8796	0.066*
C16	0.3837 (3)	0.0757 (3)	0.6328 (3)	0.0812 (8)
H16A	0.4063	0.0662	0.5487	0.122*
H16B	0.2907	0.1090	0.6377	0.122*
H16C	0.3767	-0.0135	0.6297	0.122*
C17	0.4849 (4)	0.2374 (4)	0.9569 (3)	0.1001 (10)
H17A	0.4744	0.1524	0.9619	0.150*
H17B	0.3928	0.2732	0.9569	0.150*
H17C	0.5624	0.3050	1.0376	0.150*
C18	0.7121 (3)	0.1391 (3)	0.7877 (3)	0.0899 (9)
H18A	0.7028	0.0478	0.7796	0.135*
H18B	0.7869	0.2023	0.8737	0.135*
H18C	0.7403	0.1344	0.7076	0.135*
O1	0.9113 (3)	0.6314 (2)	0.9603 (2)	0.1024 (7)
H1A	0.9910	0.6000	0.9420	0.154*
H1B	0.9090	0.6350	1.0380	0.154*
Cl1	1.14370 (9)	0.44812 (10)	0.80296 (8)	0.0961 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0616 (4)	0.0668 (4)	0.0477 (3)	0.0106 (3)	0.0191 (3)	0.0301 (3)
N1	0.0349 (8)	0.0565 (9)	0.0533 (9)	0.0048 (7)	0.0145 (7)	0.0295 (8)
N2	0.0448 (9)	0.0524 (9)	0.0460 (8)	0.0074 (7)	0.0162 (7)	0.0251 (7)
C1	0.0401 (9)	0.0458 (9)	0.0466 (9)	0.0086 (7)	0.0162 (8)	0.0238 (8)
C2	0.0404 (10)	0.0611 (12)	0.0632 (12)	0.0110 (9)	0.0240 (9)	0.0324 (10)
C3	0.0358 (10)	0.0717 (14)	0.0673 (13)	0.0081 (9)	0.0120 (9)	0.0339 (11)
C4	0.0471 (12)	0.0770 (14)	0.0527 (11)	0.0088 (10)	0.0087 (9)	0.0333 (11)
C5	0.0486 (11)	0.0686 (13)	0.0516 (11)	0.0106 (9)	0.0193 (9)	0.0340 (10)
C6	0.0343 (9)	0.0484 (10)	0.0507 (10)	0.0068 (7)	0.0145 (8)	0.0260 (8)
C7	0.0418 (10)	0.0554 (11)	0.0511 (11)	0.0031 (8)	0.0079 (8)	0.0260 (9)
C8	0.0360 (10)	0.0667 (13)	0.0736 (13)	0.0050 (9)	0.0216 (9)	0.0412 (11)
C9	0.0311 (9)	0.0671 (12)	0.0673 (12)	0.0090 (8)	0.0197 (9)	0.0400 (10)
C10	0.0529 (13)	0.1023 (19)	0.0737 (15)	0.0312 (13)	0.0236 (12)	0.0498 (15)
C11	0.0647 (17)	0.126 (3)	0.0702 (17)	0.0308 (17)	0.0212 (14)	0.0299 (17)
C12	0.0684 (18)	0.0793 (19)	0.120 (3)	0.0195 (15)	0.0432 (18)	0.0266 (18)
C13	0.087 (2)	0.088 (2)	0.146 (3)	0.0402 (16)	0.069 (2)	0.077 (2)
C14	0.0671 (15)	0.0864 (17)	0.0943 (18)	0.0279 (13)	0.0444 (14)	0.0631 (15)
C15	0.0599 (12)	0.0622 (12)	0.0420 (10)	0.0129 (10)	0.0203 (9)	0.0217 (9)
C16	0.0781 (18)	0.0771 (17)	0.0790 (17)	−0.0077 (13)	0.0151 (14)	0.0347 (14)
C17	0.142 (3)	0.111 (2)	0.0703 (17)	0.022 (2)	0.0513 (19)	0.0526 (17)
C18	0.0818 (19)	0.093 (2)	0.088 (2)	0.0247 (16)	0.0135 (16)	0.0423 (17)
O1	0.1114 (17)	0.0974 (15)	0.0822 (13)	0.0288 (13)	0.0144 (12)	0.0355 (12)
Cl1	0.0818 (5)	0.1278 (7)	0.0780 (5)	0.0348 (4)	0.0259 (4)	0.0465 (4)

Geometric parameters (Å, °)

Si1—C18	1.834 (3)	C9—C10	1.378 (3)
Si1—C17	1.850 (3)	C9—C14	1.383 (3)
Si1—C16	1.852 (3)	C10—C11	1.380 (4)
Si1—C15	1.890 (2)	C10—H10	0.9300
N1—C7	1.328 (3)	C11—C12	1.368 (5)
N1—C6	1.386 (2)	C11—H11	0.9300
N1—C8	1.476 (2)	C12—C13	1.367 (5)
N2—C7	1.324 (2)	C12—H12	0.9300
N2—C1	1.387 (2)	C13—C14	1.376 (4)
N2—C15	1.478 (2)	C13—H13	0.9300
C1—C2	1.389 (3)	C14—H14	0.9300
C1—C6	1.394 (2)	C15—H15A	0.9700
C2—C3	1.374 (3)	C15—H15B	0.9700
C2—H2	0.9300	C16—H16A	0.9600
C3—C4	1.398 (3)	C16—H16B	0.9600
C3—H3	0.9300	C16—H16C	0.9600
C4—C5	1.369 (3)	C17—H17A	0.9600
C4—H4	0.9300	C17—H17B	0.9600
C5—C6	1.384 (3)	C17—H17C	0.9600

supplementary materials

C5—H5	0.9300	C18—H18A	0.9600
C7—H7	0.9300	C18—H18B	0.9600
C8—C9	1.497 (3)	C18—H18C	0.9600
C8—H8A	0.9700	O1—H1A	0.8598
C8—H8B	0.9700	O1—H1B	0.8466
C18—Si1—C17	111.82 (16)	C14—C9—C8	120.0 (2)
C18—Si1—C16	110.58 (15)	C9—C10—C11	120.5 (3)
C17—Si1—C16	110.93 (16)	C9—C10—H10	119.8
C18—Si1—C15	107.44 (14)	C11—C10—H10	119.8
C17—Si1—C15	105.86 (13)	C12—C11—C10	120.2 (3)
C16—Si1—C15	110.04 (12)	C12—C11—H11	119.9
C7—N1—C6	108.20 (15)	C10—C11—H11	119.9
C7—N1—C8	125.70 (17)	C13—C12—C11	119.7 (3)
C6—N1—C8	126.08 (16)	C13—C12—H12	120.1
C7—N2—C1	108.16 (15)	C11—C12—H12	120.1
C7—N2—C15	126.39 (17)	C12—C13—C14	120.4 (3)
C1—N2—C15	125.43 (16)	C12—C13—H13	119.8
N2—C1—C2	131.97 (17)	C14—C13—H13	119.8
N2—C1—C6	106.56 (16)	C13—C14—C9	120.4 (3)
C2—C1—C6	121.45 (18)	C13—C14—H14	119.8
C3—C2—C1	116.40 (18)	C9—C14—H14	119.8
C3—C2—H2	121.8	N2—C15—Si1	113.64 (13)
C1—C2—H2	121.8	N2—C15—H15A	108.8
C2—C3—C4	122.03 (19)	Si1—C15—H15A	108.8
C2—C3—H3	119.0	N2—C15—H15B	108.8
C4—C3—H3	119.0	Si1—C15—H15B	108.8
C5—C4—C3	121.6 (2)	H15A—C15—H15B	107.7
C5—C4—H4	119.2	Si1—C16—H16A	109.5
C3—C4—H4	119.2	Si1—C16—H16B	109.5
C4—C5—C6	116.92 (18)	H16A—C16—H16B	109.5
C4—C5—H5	121.5	Si1—C16—H16C	109.5
C6—C5—H5	121.5	H16A—C16—H16C	109.5
C5—C6—N1	131.92 (17)	H16B—C16—H16C	109.5
C5—C6—C1	121.62 (17)	Si1—C17—H17A	109.5
N1—C6—C1	106.41 (16)	Si1—C17—H17B	109.5
N2—C7—N1	110.68 (17)	H17A—C17—H17B	109.5
N2—C7—H7	124.7	Si1—C17—H17C	109.5
N1—C7—H7	124.7	H17A—C17—H17C	109.5
N1—C8—C9	112.22 (16)	H17B—C17—H17C	109.5
N1—C8—H8A	109.2	Si1—C18—H18A	109.5
C9—C8—H8A	109.2	Si1—C18—H18B	109.5
N1—C8—H8B	109.2	H18A—C18—H18B	109.5
C9—C8—H8B	109.2	Si1—C18—H18C	109.5
H8A—C8—H8B	107.9	H18A—C18—H18C	109.5
C10—C9—C14	118.7 (2)	H18B—C18—H18C	109.5
C10—C9—C8	121.3 (2)	H1A—O1—H1B	107.0
C7—N2—C1—C2	-178.0 (2)	C15—N2—C7—N1	178.44 (17)
C15—N2—C1—C2	3.6 (3)	C6—N1—C7—N2	-0.3 (2)

C7—N2—C1—C6	0.1 (2)	C8—N1—C7—N2	178.18 (18)
C15—N2—C1—C6	-178.27 (17)	C7—N1—C8—C9	109.6 (2)
N2—C1—C2—C3	178.1 (2)	C6—N1—C8—C9	-72.2 (2)
C6—C1—C2—C3	0.2 (3)	N1—C8—C9—C10	108.7 (2)
C1—C2—C3—C4	-0.6 (3)	N1—C8—C9—C14	-72.5 (2)
C2—C3—C4—C5	0.4 (4)	C14—C9—C10—C11	2.3 (4)
C3—C4—C5—C6	0.2 (3)	C8—C9—C10—C11	-178.8 (2)
C4—C5—C6—N1	-177.7 (2)	C9—C10—C11—C12	-0.5 (4)
C4—C5—C6—C1	-0.6 (3)	C10—C11—C12—C13	-1.5 (5)
C7—N1—C6—C5	177.7 (2)	C11—C12—C13—C14	1.7 (5)
C8—N1—C6—C5	-0.7 (3)	C12—C13—C14—C9	0.2 (4)
C7—N1—C6—C1	0.3 (2)	C10—C9—C14—C13	-2.2 (3)
C8—N1—C6—C1	-178.13 (17)	C8—C9—C14—C13	179.0 (2)
N2—C1—C6—C5	-177.97 (18)	C7—N2—C15—Si1	-91.7 (2)
C2—C1—C6—C5	0.4 (3)	C1—N2—C15—Si1	86.4 (2)
N2—C1—C6—N1	-0.2 (2)	C18—Si1—C15—N2	60.61 (19)
C2—C1—C6—N1	178.10 (18)	C17—Si1—C15—N2	-179.77 (18)
C1—N2—C7—N1	0.1 (2)	C16—Si1—C15—N2	-59.84 (19)

Hydrogen-bond geometry (Å, °)

Cg3 is the centroid of the C9–C14 ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1A...C11	0.86	2.45	3.257 (2)	157
O1—H1B...C11 ⁱ	0.85	2.45	3.250 (3)	158
C7—H7...O1	0.93	2.51	3.170 (3)	128
C8—H8A...C11	0.97	2.81	3.703 (2)	153
C3—H3...Cg3 ⁱⁱ	0.93	2.69	3.526 (2)	151

Symmetry codes: (i) $-x+2, -y+1, -z+2$; (ii) $x-1, y, z$.

Table 2

π - π stacking in the title compound (Å, °).

Cg1 is the centroid of the N1, C6, C1, N2, C7 ring and Cg2 is the centroid of C1 to C6 ring. Offset is the angle between the centroid-to-centroid and plane-to-plane vectors.

	Centroid-centroid	plane-plane	offset
Cg1...Cg2 ⁱ	3.5690 (15)	3.430 (1)	16.0
Cg2...Cg2 ⁱ	3.7223 (14)	3.446 (1)	22.2

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

Fig. 1

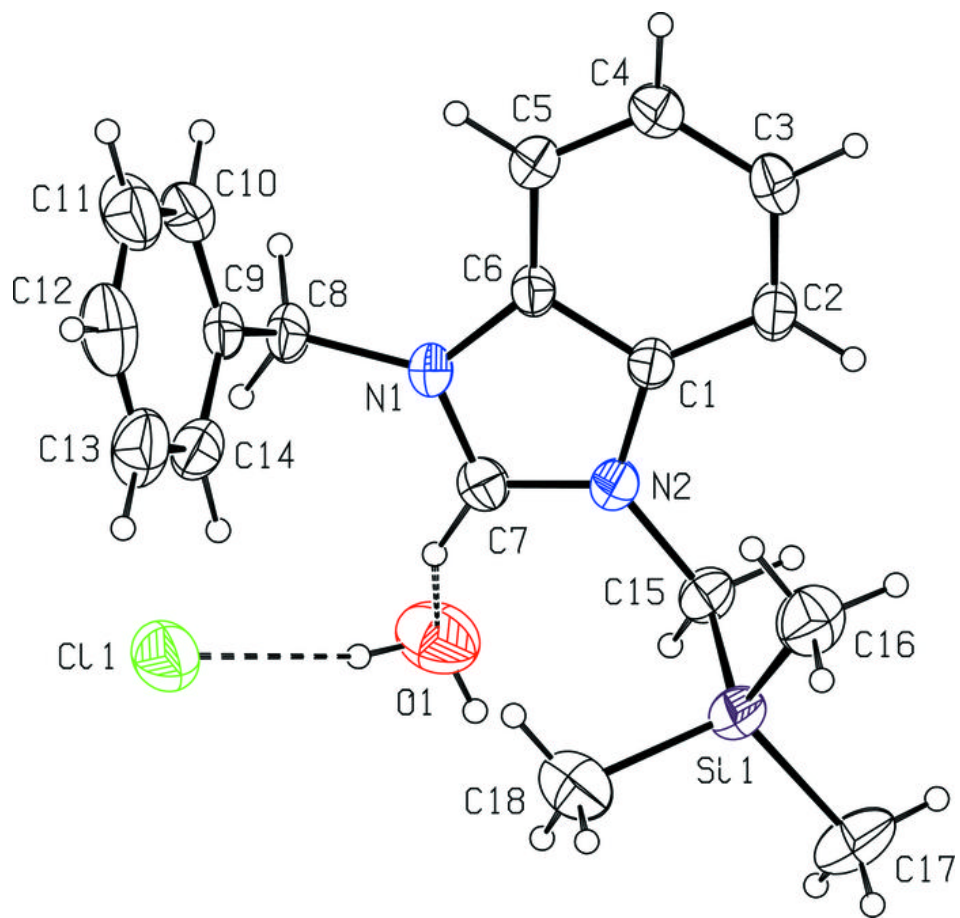


Fig. 2

