

1-(Prop-2-en-1-yl)-3-[(trimethylsilyl)methyl]benzimidazolium bromide monohydrate

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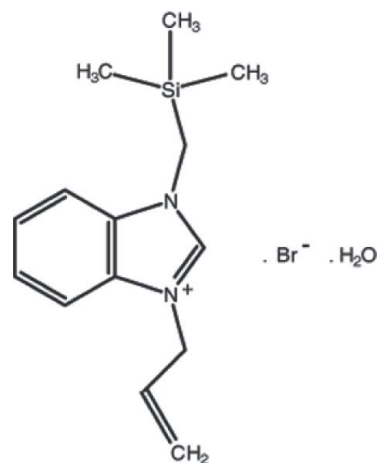
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Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.049; wR factor = 0.121; data-to-parameter ratio = 20.7.

In the title compound, $\text{C}_{14}\text{H}_{21}\text{N}_2\text{Si}^+\cdot\text{Br}^-\cdot\text{H}_2\text{O}$, the benzimidazole ring system is almost planar [maximum deviation = 0.021 (2) Å]. In the crystal, $\text{O}-\text{H}\cdots\text{Br}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the ions *via* the O atoms of the water molecules. In addition, there are $\pi-\pi$ stacking interactions between the centroids of the benzene and imidazole rings of the benzimidazole ring system [centroid-centroid distances = 3.521 (3) and 3.575 (2) Å].

Related literature

For the antitumour activity of alkylsilyl-substituted benzimidazole derivatives, see: Kleemann *et al.* (2009); Lukevics *et al.* (2001); Ignatovich *et al.* (2010). For the pharmacological activity of benzimidazole compounds, see: Singh & Lown (2000); Huang *et al.* (2006); Turner & Denny (1996); Galal *et al.* (2009); Küçükbay *et al.* (2003, 2004, 2009, 2010a,b); Şireci *et al.* (2010); Yılmaz & Küçükbay (2009); Yılmaz *et al.* (2010). For the structures of similar benzimidazole derivatives, see: Akkurt *et al.* (2008, 2010a,b); Yıldırım *et al.* (2006). For $\pi-\pi$ interactions, see: Janiak (2000).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{21}\text{N}_2\text{Si}^+\cdot\text{Br}^-\cdot\text{H}_2\text{O}$
 $M_r = 343.33$
 Triclinic, $P\bar{1}$
 $a = 8.9063$ (2) Å
 $b = 10.4720$ (2) Å
 $c = 10.9439$ (3) Å
 $\alpha = 66.542$ (4)°
 $\beta = 71.479$ (4)°
 $\gamma = 80.625$ (5)°
 $V = 887.07$ (5) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 2.38$ mm⁻¹
 $T = 294$ K
 $0.20 \times 0.20 \times 0.20$ mm

Data collection

Rigaku R-Axis RAPID-S diffractometer
 Absorption correction: multi-scan (SORTAV; Blessing, 1995)
 $T_{\min} = 0.647$, $T_{\max} = 0.647$
 18957 measured reflections
 3618 independent reflections
 2202 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.073$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.121$
 $S = 1.02$
 3618 reflections
 175 parameters
 3 restraints
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.30$ e Å⁻³
 $\Delta\rho_{\min} = -0.35$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C7}-\text{H7}\cdots\text{O1W}$	0.93	2.46	3.351 (5)	161
$\text{O1W}-\text{H1W}\cdots\text{Br1}$	0.85	2.62	3.445 (4)	165
$\text{O1W}-\text{H2W}\cdots\text{Br1}^1$	0.85	2.59	3.360 (4)	152

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

Data collection: *CrystalClear* (Rigaku/MS, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *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: DN2597).

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supporting information

Acta Cryst. (2010). E66, o2393–o2394 [https://doi.org/10.1107/S1600536810033015]

1-(Prop-2-en-1-yl)-3-[(trimethylsilyl)methyl]benzimidazolium bromide monohydrate

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S1. Comment

Heterocycles are important building blocks for the construction of anticancer drugs (Kleemann *et al.*, 2009). For example, alkylsilyl substituted benzimidazole derivatives have been reported to possess important antitumour activity (Lukevics *et al.*, 2001; Ignatovich *et al.*, 2010). 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 & Lown, 2000; Huang *et al.*, 2006; Turner & Denny, 1996; Galal *et al.*, 2009; Küçükbay *et al.*, 2003, 2004, 2009, 2010*a,b*; Şireci *et al.*, 2010; Yılmaz *et al.*, 2009, 2010;). We have synthesized and investigated the crystal structures of many benzimidazole derivatives (Akkurt *et al.*, 2008, 2010*a,b*; Yıldırım *et al.*, 2006). Herein we report the synthesis and structure of the title compound, (I), 1-(prop-2-ene-1-yl)-3-[(trimethylsilyl)methyl]benzimidazolium bromide monohydrate.

The benzimidazole ring system (N1/N2/C1–C7) in the title molecule (I) (Fig. 1) is almost planar with a maximum deviation of 0.021 (2) Å for C1 atom. The bond lengths and angles in (I) are compatible with those found for similar compounds (Akkurt *et al.*, 2008, 2010*a,b*). The average Si—C bond length is 1.857 (5) Å. The angles around the Si atoms with a distorted tetrahedral geometry vary from 105.9 (2)° to 111.7 (3)°.

O—H···Br and C—H···O hydrogen bonds link the molecules (Table 1 and Fig 2). In the crystal structure, the benzene (C1–C6) and imidazole (N1/N2/C1/C6/C7) rings of the benzimidazole ring system form π - π stacking interactions with each other (Janiak, 2000) (Table 2).

S2. Experimental

A mixture of 1-(trimethylsilylmethyl)benzimidazole (1.02 g, 4.99 mmol) and allyl bromide (0.5 ml, 5.78 mmol) in dimethylformamide (5 ml) was refluxed for 3 h. The mixture was then cooled and the volatiles were removed under vacuum. The residue was crystallized from a dimethylformamide/ethanol (1:1). White crystals of the title compound (1.29 g, 79%) were obtained, m.p.: 394–395 °K; $\nu_{(\text{CN})}$ = 1552 cm^{-1} . Anal. found: C 48.67, H 6.72, N 8.11%. Calculated for $\text{C}_{14}\text{H}_{23}\text{BrN}_2\text{OSi}$: C 48.98, H 6.75, N 8.16%. ^1H NMR (δ , DMSO- d_6): 9.70 (s, 1H, NCHN), 8.14 - 7.67 (m, 4H, C_6H_4), 6.12 (m, 1H, CH allyl), 5.37 (m, 2H, CH_2 allyl), 5.22 (d, 2H, CH_2 allyl, $J = 5.7$ Hz), 4.26 (s, 2H, CH_2Si) and 0.11 [s, 9H, $(\text{CH}_3)_3\text{Si}$]. ^{13}C NMR (δ , DMSO- d_6): 141.6 (NCHN), 132.5, 131.9, 131.3, 127.0, 126.8 and 120.4 (C_6H_4), 114.5 (CH allyl), 114.2 (CH_2 allyl), 49.2 (CH_2 allyl), 38.4 (CH_2Si) and -2.2 [$(\text{CH}_3)_3\text{Si}$].

S3. Refinement

The hydrogen atoms on the water molecule were located from a difference Fourier map and refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å, and with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$. In the last steps of refinement, they were treated as riding on the parent O atom. The other H atoms were positioned geometrically, with C—H = 0.93–0.97 Å,

and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5 U_{\text{eq}}(\text{C})$.

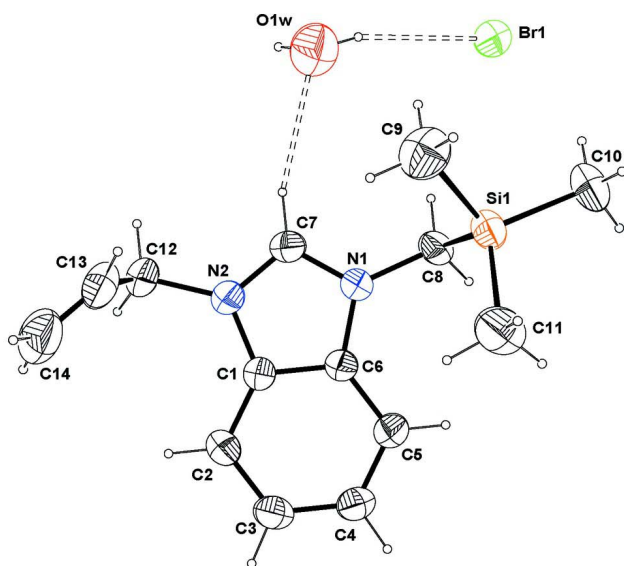


Figure 1

View of the title molecule 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. Hydrogen bonds are shown as dashed lines.

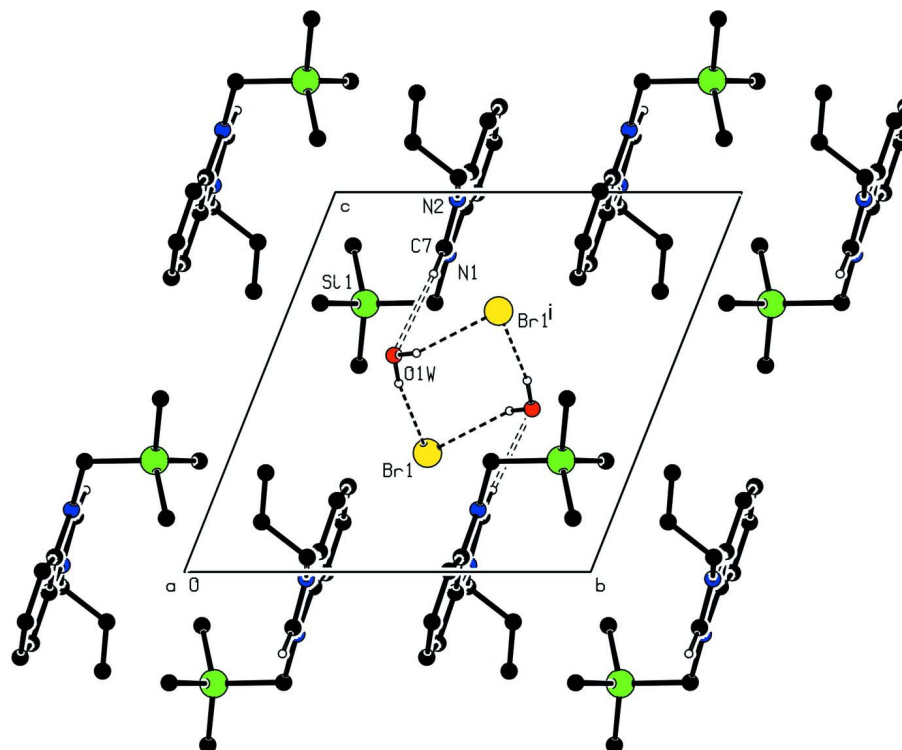


Figure 2

Packing view of the title compound with O—H \cdots Br and C—H \cdots O hydrogen bonds viewed down the *a* axis. H atoms not involved in hydrogen bondings are omitted for the sake of clarity. [Symmetry code: (i) $-x+2, -y+1, -z+1$]

1-(Prop-2-en-1-yl)-3-[(trimethylsilyl)methyl]benzimidazolium bromide monohydrate

Crystal data

$C_{14}H_{21}N_2Si^+ \cdot Br^- \cdot H_2O$

$M_r = 343.33$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.9063\ (2)\ \text{\AA}$

$b = 10.4720\ (2)\ \text{\AA}$

$c = 10.9439\ (3)\ \text{\AA}$

$\alpha = 66.542\ (4)^\circ$

$\beta = 71.479\ (4)^\circ$

$\gamma = 80.625\ (5)^\circ$

$V = 887.07\ (5)\ \text{\AA}^3$

$Z = 2$

$F(000) = 356$

$D_x = 1.285\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3185 reflections

$\theta = 2.4\text{--}26.4^\circ$

$\mu = 2.38\ \text{mm}^{-1}$

$T = 294\ \text{K}$

Block, white

$0.20 \times 0.20 \times 0.20\ \text{mm}$

Data collection

Rigaku R-AXIS RAPID-S

diffractometer

Radiation source: Sealed Tube

Graphite Monochromator monochromator

Detector resolution: $10.0000\ \text{pixels mm}^{-1}$

dtprofit.ref scans

Absorption correction: multi-scan

(*SORTAV*; Blessing, 1995)

$T_{\min} = 0.647, T_{\max} = 0.647$

18957 measured reflections

3618 independent reflections

2202 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.073$

$\theta_{\max} = 26.4^\circ, \theta_{\min} = 2.4^\circ$

$h = -11 \rightarrow 9$

$k = -13 \rightarrow 13$

$l = -13 \rightarrow 13$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.049$ $wR(F^2) = 0.121$ $S = 1.02$

3618 reflections

175 parameters

3 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 0.3659P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.006$ $\Delta\rho_{\max} = 0.30 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.35 \text{ e } \text{\AA}^{-3}$ *Special details***Geometry.** Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles**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	0.53721 (14)	0.18235 (12)	0.70600 (11)	0.0684 (3)
N1	0.6155 (3)	0.3381 (3)	0.8362 (3)	0.0570 (7)
N2	0.7515 (3)	0.3069 (3)	0.9818 (3)	0.0624 (8)
C1	0.5921 (4)	0.3128 (4)	1.0536 (4)	0.0562 (9)
C2	0.5185 (5)	0.3059 (4)	1.1879 (4)	0.0669 (10)
H2	0.5760	0.2927	1.2499	0.080*
C3	0.3555 (5)	0.3197 (4)	1.2249 (4)	0.0722 (11)
H3	0.3016	0.3143	1.3147	0.087*
C4	0.2689 (5)	0.3415 (4)	1.1314 (4)	0.0673 (10)
H4	0.1590	0.3509	1.1604	0.081*
C5	0.3419 (4)	0.3495 (4)	0.9978 (4)	0.0625 (9)
H5	0.2844	0.3649	0.9353	0.075*
C6	0.5059 (4)	0.3332 (4)	0.9609 (3)	0.0546 (8)
C7	0.7597 (4)	0.3221 (4)	0.8533 (4)	0.0634 (10)
H7	0.8535	0.3216	0.7846	0.076*
C8	0.5773 (5)	0.3529 (4)	0.7092 (3)	0.0634 (10)
H8A	0.6649	0.3954	0.6294	0.076*
H8B	0.4847	0.4153	0.7007	0.076*
C9	0.7201 (6)	0.0716 (5)	0.7079 (6)	0.1093 (17)
H9A	0.7050	-0.0136	0.7007	0.164*
H9B	0.7453	0.0508	0.7931	0.164*
H9C	0.8055	0.1197	0.6310	0.164*
C10	0.4835 (6)	0.2278 (6)	0.5440 (5)	0.1070 (17)
H10A	0.3868	0.2840	0.5472	0.160*
H10B	0.4690	0.1442	0.5337	0.160*

H10C	0.5666	0.2790	0.4667	0.160*
C11	0.3721 (6)	0.0963 (5)	0.8586 (5)	0.1049 (16)
H11A	0.3672	0.0022	0.8668	0.157*
H11B	0.2741	0.1463	0.8470	0.157*
H11C	0.3897	0.0958	0.9409	0.157*
C12	0.8871 (5)	0.2883 (5)	1.0387 (4)	0.0781 (12)
H12A	0.8701	0.3488	1.0902	0.094*
H12B	0.9831	0.3152	0.9629	0.094*
C13	0.9078 (5)	0.1417 (5)	1.1316 (6)	0.0889 (14)
H13	0.9301	0.0731	1.0937	0.107*
C14	0.8967 (6)	0.1037 (6)	1.2611 (7)	0.1190 (19)
H14A	0.8744	0.1698	1.3021	0.143*
H14B	0.9109	0.0101	1.3139	0.143*
O1W	1.0389 (5)	0.3039 (4)	0.5704 (4)	0.1283 (12)
H1W	1.0104	0.3435	0.4962	0.192*
H2W	1.0969	0.3573	0.5761	0.192*
Br1	0.85464 (5)	0.48204 (5)	0.31301 (5)	0.0895 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Si1	0.0770 (8)	0.0756 (7)	0.0588 (6)	-0.0017 (6)	-0.0259 (6)	-0.0264 (6)
N1	0.0539 (18)	0.067 (2)	0.0517 (17)	-0.0005 (14)	-0.0141 (14)	-0.0253 (15)
N2	0.0522 (18)	0.076 (2)	0.065 (2)	-0.0021 (15)	-0.0165 (15)	-0.0321 (17)
C1	0.052 (2)	0.064 (2)	0.055 (2)	-0.0033 (17)	-0.0155 (17)	-0.0241 (18)
C2	0.071 (3)	0.080 (3)	0.055 (2)	-0.005 (2)	-0.018 (2)	-0.029 (2)
C3	0.072 (3)	0.082 (3)	0.059 (2)	-0.007 (2)	-0.005 (2)	-0.030 (2)
C4	0.054 (2)	0.073 (3)	0.072 (3)	-0.0029 (19)	-0.008 (2)	-0.031 (2)
C5	0.055 (2)	0.066 (2)	0.066 (2)	0.0009 (18)	-0.0174 (19)	-0.0259 (19)
C6	0.052 (2)	0.061 (2)	0.053 (2)	-0.0012 (16)	-0.0122 (17)	-0.0258 (17)
C7	0.053 (2)	0.076 (3)	0.062 (2)	-0.0019 (18)	-0.0085 (18)	-0.032 (2)
C8	0.069 (2)	0.072 (3)	0.045 (2)	-0.0009 (19)	-0.0158 (18)	-0.0188 (18)
C9	0.107 (4)	0.087 (3)	0.137 (5)	0.015 (3)	-0.043 (3)	-0.044 (3)
C10	0.121 (4)	0.144 (5)	0.079 (3)	-0.010 (3)	-0.041 (3)	-0.053 (3)
C11	0.120 (4)	0.103 (4)	0.090 (3)	-0.039 (3)	-0.011 (3)	-0.035 (3)
C12	0.056 (2)	0.107 (4)	0.085 (3)	-0.005 (2)	-0.027 (2)	-0.042 (3)
C13	0.067 (3)	0.099 (4)	0.115 (4)	0.009 (2)	-0.044 (3)	-0.044 (3)
C14	0.098 (4)	0.117 (5)	0.130 (5)	0.009 (3)	-0.055 (4)	-0.022 (4)
O1W	0.124 (3)	0.130 (3)	0.132 (3)	-0.002 (2)	-0.047 (2)	-0.042 (2)
Br1	0.0699 (3)	0.1215 (4)	0.0769 (3)	0.0007 (3)	-0.0195 (2)	-0.0391 (3)

Geometric parameters (Å, °)

Si1—C9	1.840 (5)	C8—H8A	0.9700
Si1—C10	1.842 (4)	C8—H8B	0.9700
Si1—C11	1.854 (5)	C9—H9A	0.9600
Si1—C8	1.893 (4)	C9—H9B	0.9600
N1—C7	1.329 (4)	C9—H9C	0.9600

N1—C6	1.390 (4)	C10—H10A	0.9600
N1—C8	1.478 (4)	C10—H10B	0.9600
N2—C7	1.330 (4)	C10—H10C	0.9600
N2—C1	1.392 (4)	C11—H11A	0.9600
N2—C12	1.480 (5)	C11—H11B	0.9600
C1—C2	1.383 (5)	C11—H11C	0.9600
C1—C6	1.390 (5)	C12—C13	1.486 (6)
C2—C3	1.377 (5)	C12—H12A	0.9700
C2—H2	0.9300	C12—H12B	0.9700
C3—C4	1.397 (5)	C13—C14	1.285 (7)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.372 (5)	C14—H14A	0.9300
C4—H4	0.9300	C14—H14B	0.9300
C5—C6	1.387 (5)	O1W—H1W	0.8512
C5—H5	0.9300	O1W—H2W	0.8513
C7—H7	0.9300		
C9—Si1—C10	111.7 (2)	Si1—C8—H8A	108.8
C9—Si1—C11	110.6 (2)	N1—C8—H8B	108.8
C10—Si1—C11	110.6 (2)	Si1—C8—H8B	108.8
C9—Si1—C8	107.8 (2)	H8A—C8—H8B	107.7
C10—Si1—C8	105.9 (2)	Si1—C9—H9A	109.5
C11—Si1—C8	110.15 (19)	Si1—C9—H9B	109.5
C7—N1—C6	108.0 (3)	H9A—C9—H9B	109.5
C7—N1—C8	126.3 (3)	Si1—C9—H9C	109.5
C6—N1—C8	125.7 (3)	H9A—C9—H9C	109.5
C7—N2—C1	107.9 (3)	H9B—C9—H9C	109.5
C7—N2—C12	126.3 (3)	Si1—C10—H10A	109.5
C1—N2—C12	125.8 (3)	Si1—C10—H10B	109.5
C2—C1—C6	121.7 (3)	H10A—C10—H10B	109.5
C2—C1—N2	131.6 (3)	Si1—C10—H10C	109.5
C6—C1—N2	106.7 (3)	H10A—C10—H10C	109.5
C3—C2—C1	116.5 (3)	H10B—C10—H10C	109.5
C3—C2—H2	121.8	Si1—C11—H11A	109.5
C1—C2—H2	121.8	Si1—C11—H11B	109.5
C2—C3—C4	121.9 (4)	H11A—C11—H11B	109.5
C2—C3—H3	119.0	Si1—C11—H11C	109.5
C4—C3—H3	119.0	H11A—C11—H11C	109.5
C5—C4—C3	121.7 (4)	H11B—C11—H11C	109.5
C5—C4—H4	119.2	N2—C12—C13	111.7 (3)
C3—C4—H4	119.2	N2—C12—H12A	109.3
C4—C5—C6	116.6 (3)	C13—C12—H12A	109.3
C4—C5—H5	121.7	N2—C12—H12B	109.3
C6—C5—H5	121.7	C13—C12—H12B	109.3
C5—C6—N1	131.6 (3)	H12A—C12—H12B	107.9
C5—C6—C1	121.7 (3)	C14—C13—C12	124.1 (5)
N1—C6—C1	106.7 (3)	C14—C13—H13	118.0
N2—C7—N1	110.8 (3)	C12—C13—H13	118.0

N2—C7—H7	124.6	C13—C14—H14A	120.0
N1—C7—H7	124.6	C13—C14—H14B	120.0
N1—C8—Si1	113.9 (2)	H14A—C14—H14B	120.0
N1—C8—H8A	108.8	H1W—O1W—H2W	109.9

Hydrogen-bond geometry (Å, °)

<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>
C7—H7...O1 <i>W</i>	0.93	2.46	3.351 (5)	161
O1 <i>W</i> —H1 <i>W</i> ...Br1	0.85	2.62	3.445 (4)	165
O1 <i>W</i> —H2 <i>W</i> ...Br1 ⁱ	0.85	2.59	3.360 (4)	152

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