Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Zeliha Baktır,[a] Mehmet Akkurt,[a]* Nihat Şireci[b] and Hasan Küçükbay[c]

[a]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, [b]Department of Chemistry, Faculty of Arts and Sciences, Adıyaman University, 02040 Adıyaman, Turkey, and [c]Department of Chemistry, Faculty of Arts and Sciences, İnönü University, 44280 Malatya, Turkey
Correspondence e-mail: akkurt@erciyes.edu.tr

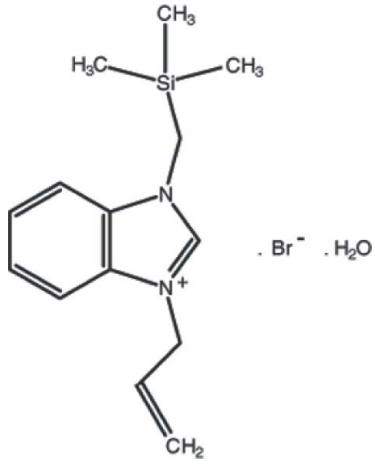
Received 12 August 2010; accepted 16 August 2010

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.006 Å; R factor = 0.049; wR factor = 0.121; data-to-parameter ratio = 20.7.

In the title compound, $C_{14}H_{21}N_2Si^+\cdot Br^-\cdot H_2O$, the benzimidazole ring system is almost planar [maximum deviation = 0.021 (2) Å]. In the crystal, O—H···Br and C—H···O hydrogen bonds link the ions *via* the O atoms of the water molecules. In addition, there are π–π 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, 2010*a*,*b*); Şireci *et al.* (2010); Yılmaz & Küçükbay (2009); Yılmaz *et al.* (2010). For the structures of similar benzimidazole derivatives, see: Akkurt *et al.* (2008, 2010*a*,*b*); Yıldırım *et al.* (2006). For π–π interactions, see: Janiak (2000).



Experimental

Crystal data

$C_{14}H_{21}N_2Si^+\cdot Br^-\cdot H_2O$
M_r = 343.33
Triclinic, $P\overline{1}$
a = 8.9063 (2) Å
b = 10.4720 (2) Å
c = 10.9439 (3) Å
α = 66.542 (4)°
β = 71.479 (4)°
γ = 80.625 (5)°
V = 887.07 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.38 mm^{-1}
T = 294 K
0.20 × 0.20 × 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_{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—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O1W	0.93	2.46	3.351 (5)	161
O1W—H1W···Br1	0.85	2.62	3.445 (4)	165
O1W—H2W···Br1^{i}	0.85	2.59	3.360 (4)	152

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

Data collection: *CrystalClear* (Rigaku/MSC, 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).

ZB and MA thank the Unit of the Scientific Research Projects of Erciyes University, Turkey for the research grant FBD-10–2949, and for support of the data collection at

Atatürk University, Turkey. HK and NŞ thank İnönü University Research Fund (BAPB-2008–60) for financial support of this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2597).

References

Akkurt, M., Çelik, Í., Küçükbay, H., Şireci, N. & Büyükgüngör, O. (2010*a*). *Acta Cryst.* E**66**, o1770–o1771.

Akkurt, M., Karaca, S., Küçükbay, H., Şireci, N. & Büyükgüngör, O. (2008). *Acta Cryst.* E**64**, o809.

Akkurt, M., Yalçın, Ş. P., Şireci, N., Küçükbay, H. & Tahir, M. N. (2010*b*). *Acta Cryst.* E**66**, m253–m254.

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Galal, S. A., Hegab, K. H., Kassab, A. S., Rodriguez, M. L., Kerwin, S. M., El-Khamry, A.-M. A. & Divani, H. I. E. (2009). *Eur. J. Med. Chem.* **44**, 1500–1508.

Huang, S.-T., Hsei, I.-J. & Chen, C. (2006). *Bioorg. Med. Chem.* **14**, 6106–6119.

Ignatovich, I., Muravenko, V., Shestakova, I., Domrachova, I., Popelis, J. & Lukevics, E. (2010). *Appl. Organomet. Chem.* **24**, 158–161.

Janiak, C. (2000). *J. Chem. Soc. Dalton Trans.* pp. 3885–3896.

Kleemann, A., Engel, J., Kutscher, B. & Reichert, D. (2009). *Pharmaceutical Substances*. Stuttgard, Germany: Thieme.

Küçükbay, H., Durmaz, R., Okuyucu, N. & Günal, S. (2003). *Fol. Microbiol.* **48**, 679–681.

Küçükbay, H., Durmaz, R., Okuyucu, N., Günal, S. & Kazaz, C. (2004). *Arzneim. Forsch. Drug Res.* **54**, 64–68.

Küçükbay, H., Durmaz, R., Şireci, N. & Günal, S. (2009). *Asian J. Chem.* **21**, 6181–6189.

Küçükbay, H., Durmaz, R., Şireci, N. & Günal, S. (2010*a*). *Asian J. Chem.* **22**, 2816–2824.

Küçükbay, H., Günal, S., Orhan, E. & Durmaz, R. (2010*b*). *Asian J. Chem.* **22**, 7376–7382.

Lukevics, E., Arsenyan, P., Shestakova, I. Domracheva, I., Nesterova, A. & Pudova, O. (2001). *Eur. J. Med. Chem.* **36**, 507–515.

Rigaku/MSC (2005). *CrystalClear*. Rigaku/MSC, The Woodlands, Texas, USA.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Singh, A. K. & Lown, J. W. (2000). *Anti-Cancer Drug Des.* **15**, 265–275.

Şireci, N., Yılmaz, Ü. & Küçükbay, H. (2010). *Asian J. Chem.* **22**, 7153–7158.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Turner, P. R. & Denny, W. A. (1996). *Mutat. Res.* **355**, 141–169.

Yıldırım, S. Ö., Akkurt, M., Yılmaz, Ü., Küçükbay, H. & McKee, V. (2006). *Acta Cryst.* E**62**, o5697–o5698.

Yılmaz, Ü. & Küçükbay, H. (2009). *Asian J. Chem.* **21**, 6149–6155.

Yılmaz, Ü., Şireci, N., Deniz, S. & Küçükbay, H. (2010). *Appl. Organomet. Chem.* **24**, 414–420.

supplementary materials

Acta Cryst. (2010). E**66**, o2393-o2394 [**doi:10.1107/S1600536810033015**]

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

Z. Baktir, M. Akkurt, N. Sireci and H. Küçükbay

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).

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; $\upsilon_{(CN)}$= 1552 cm^{-1}. Anal. found: C 48.67, H 6.72, N 8.11%. Calculated for $C_{14}H_{23}BrN_2OSi$: C 48.98, H 6.75, N 8.16%. ^{1}H 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, $(CH_3)_3Si$]. ^{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 [$(CH_3)_3Si$].

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_{iso}(H) = 1.5 U_{eq}(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_{iso}(H) = 1.2 or 1.5 U_{eq}(C).

Figures

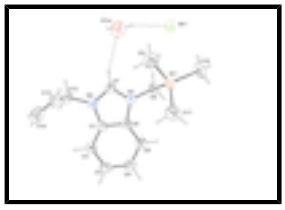


Fig. 1. View of the title molecule with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii. Hydrogen bonds are shown as dashed lines.

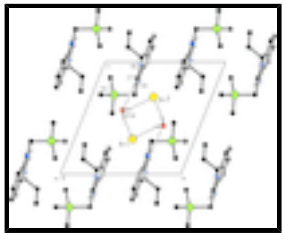


Fig. 2. Packing view of the title compound with O–H···Br and C—H···O hydrogen bonds viewed down the *a* axis. H atoms not involved in hydrogen bondings are omitted for the sake of clarity. [Symmetry code: (i) -*x*+2, -*y*+1, -*z*+1]

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

Crystal data

$C_{14}H_{21}N_2Si^+·Br^-·H_2O$	$Z = 2$
$M_r = 343.33$	$F(000) = 356$
Triclinic, $P\overline{1}$	$D_x = 1.285$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.9063$ (2) Å	Cell parameters from 3185 reflections
$b = 10.4720$ (2) Å	$\theta = 2.4$–$26.4°$
$c = 10.9439$ (3) Å	$\mu = 2.38$ mm^{-1}
$\alpha = 66.542$ (4)°	$T = 294$ K
$\beta = 71.479$ (4)°	Block, white
$\gamma = 80.625$ (5)°	0.20 × 0.20 × 0.20 mm
$V = 887.07$ (5) Å^3	

Data collection

Rigaku R-AXIS RAPID-S diffractometer	3618 independent reflections
Radiation source: Sealed Tube	2202 reflections with $I > 2\sigma(I)$
Graphite Monochromator	$R_{int} = 0.073$
Detector resolution: 10.0000 pixels mm^{-1}	$\theta_{max} = 26.4°$, $\theta_{min} = 2.4°$
dtprofit.ref scans	$h = -11 \rightarrow 9$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	$k = -13 \rightarrow 13$
$T_{min} = 0.647$, $T_{max} = 0.647$	$l = -13 \rightarrow 13$
18957 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
$wR(F^2) = 0.121$	H-atom parameters constrained
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 0.3659P]$ where $P = (F_o^2 + 2F_c^2)/3$
3618 reflections	$(\Delta/\sigma)_{max} = 0.006$
175 parameters	$\Delta\rho_{max} = 0.30$ e Å^{-3}
3 restraints	$\Delta\rho_{min} = -0.35$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{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 (Å^2)

	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, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1W	0.93	2.46	3.351 (5)	161.
O1W—H1W···Br1	0.85	2.62	3.445 (4)	165.
O1W—H2W···Br1^{i}	0.85	2.59	3.360 (4)	152.

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1.

Table 2

π-π contacts (Å, °)

Cg1: N1,N2,C1,C6,C7; Cg2: C1,C2,C3,C4,C5,C6; ccd: Distance between ring centroids; ipd: mean interplanar distance (Distance from one plane to the neighbouring centroid); sa: mean slippage angle (Angle subtended by the intercentroid vector to the plane normal). For details, see Janiak (2000).

ring 1/ring 2	ccd	ipd	sa
Cg1->Cg2^{ii}	3.521 (3)	3.386	15.9
Cg2->Cg2^{ii}	3.575 (2)	3.396	18.2

Symmetry code: (ii) 1-x,1-y,2-z.

Fig. 1

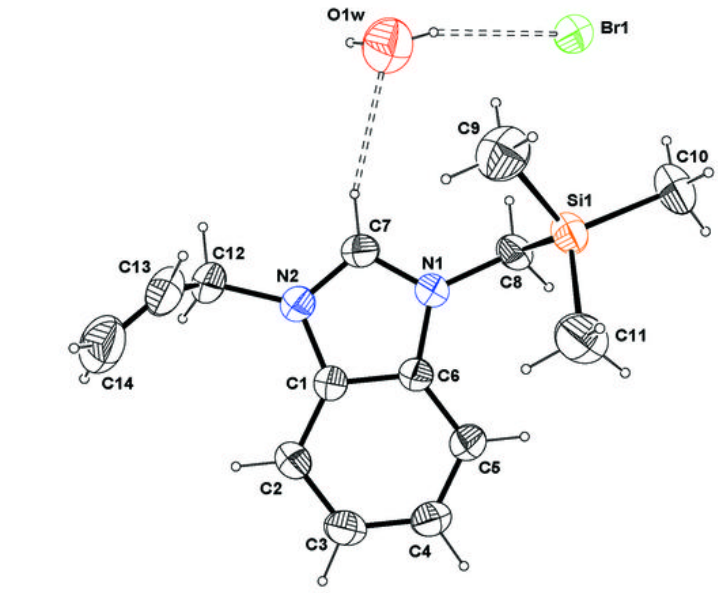


Fig. 2