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# 2-Trifluoromethyl-1*H*-benzimidazol-3-ium tetrafluoroborate–2-trifluoromethyl-1*H*-benzimidazole–water (1/1/1)

**Ming-Liang Liu**

Ordered Matter Science Research Center, Southeast University, Nanjing 211189, People's Republic of China
Correspondence e-mail: jgsdxlml@163.com

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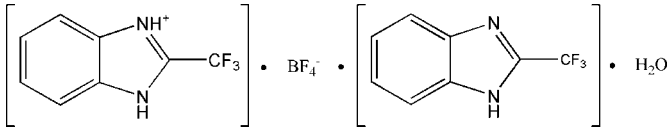
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; disorder in main residue; $R$ factor = 0.066; $wR$ factor = 0.195; data-to-parameter ratio = 12.9.

The asymmetric unit of the title compound, $C_8H_6F_3N_2^+\cdot BF_4^-\cdot C_8H_5F_3N_2\cdot H_2O$, consists of two 2-trifluoromethylbenzimidazole molecules, each of which is protonated on a 50% basis, one tetrafluoroborate anion and a water molecule. The two 2-trifluoromethylbenzimidazole molecules thus exist as half-neutral half-cation entities. They are linked by N—H···N hydrogen bonds involving the half-occupancy hydrogens in each molecule. The F atoms of one of the trifluoromethyl groups are disordered over two sets of sites [in a 0.518 (14):0.482 (14) ratio], as are the F atoms of the tetrafluoroborate anion [0.507 (14):0.493 (14) ratio]. The water molecule is linked to one of the 2-trifluoromethylbenzimidazole molecules *via* an N—H···O hydrogen bond.

## Related literature

The title compound was synthesized as part of our search for ferroelectric complexes. For background to ferroelectric complexes, see: Fu *et al.* (2011); Zhang *et al.* (2010). For related structures, see: Liu (2011*a*,*b*, 2012).



## Experimental

### Crystal data

$C_8H_6F_3N_2^+\cdot BF_4^-\cdot C_8H_5F_3N_2\cdot H_2O$
$M_r$ = 478.11
Triclinic, $P\overline{1}$
$a$ = 8.7897 (18) Å
$b$ = 10.947 (2) Å
$c$ = 11.458 (2) Å
$\alpha$ = 92.48 (3)°
$\beta$ = 96.59 (3)°
$\gamma$ = 113.34 (3)°
$V$ = 1000.8 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.17 mm$^{-1}$
$T$ = 293 K
0.36 × 0.32 × 0.28 mm

### Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.566, $T_{max}$ = 0.640
10445 measured reflections
4581 independent reflections
2280 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.195
$S$ = 1.03
4581 reflections
355 parameters
65 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N4—H4$A$···O1$W$ | 0.86 | 1.84 | 2.698 (3) | 177 |
| N1—H1···N3 | 0.86 | 1.86 | 2.718 (3) | 175 |
| N3—H3···N1 | 0.86 | 1.86 | 2.718 (3) | 175 |

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GO2047).

## References

Fu, D. W., Zhang, W., Cai, H. L., Zhang, Y., Ge, J. Z., Xiong, R. G. & Huang, S. P. (2011). *J. Am. Chem. Soc.* **133**, 12780–12786.
Liu, M.-L. (2011*a*). *Acta Cryst.* E**67**, o2821.
Liu, M.-L. (2011*b*). *Acta Cryst.* E**67**, o3473.
Liu, M.-L. (2012). *Acta Cryst.* E**68**, o342.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Zhang, W., Chen, L. Z., Gou, M., Li, Y. H., Fu, D. W. & Xiong, R. G. (2010). *Cryst. Growth Des.* **10**, 1025–1027.

# supplementary materials

*Acta Cryst.* (2012). E**68**, o1076 [doi:10.1107/S1600536812010847]

# 2-Trifluoromethyl-1*H*-benzimidazol-3-ium tetrafluoroborate–2-trifluoromethyl-1*H*-benzimidazole–water (1/1/1)

**Ming-Liang Liu**

## Comment

Recently much attention has been devoted to crystals containing organic ions and inorganic ions due to the possibility of tuning their special structural features and their potential ferroelectrics properties (Fu *et al.*, 2011; Zhang *et al.*, 2010.). In our laboratory, the title compound has been synthesized to investigate to its potentialferroelectric properties. However, it was found that the dielectric constant of the compound as a function of temperature indicates that the permittivity is basically temperature-independent ($\varepsilon = C/(T–T_0)$), suggesting that this compound is not ferroelectric or there may be no distinct phase transition occurring within the measured temperature (below the melting point).

The title compound, Figure 1, has an asymmetric unit which consists of two 2-trifluoromethylbenzimidazole molecules each of which is protonated on a 50% basis, one tetrafluoroborate anion,and a water molecule. The two trifluoromethylbenzimidazole moieties thus exist as a half neutral half cation entities. The two 2-trifluoromethylbenzimidazole molecules are hydrogen bonded together, on a 50/50 basis, by either the N1–H1···N3 or N3—H3···N1 hydrogen bonds, Table 1. One of the trifluoromethyl groups is disordered as is the tetraflouroborate anion. The water molecule is hydrogen bonded to one of the 2-trifluoromethylbenzimidazole molecules via the N4–H4A···O1W hydrogen bond Table 1. There are short N—H and O—H contacts to the F atoms of the anion but no analysis is made here because of the disorder in the anion.

## Experimental

0.144 g (1 mmol) of 2-trifluoromethyl-1*H*-benzimidazol was firstly dissolved in 30 ml of ethanol, to which 0.088 g (1 mmol) of fluoroboric acid was added to give a solution at the ambient temperature. Single crystals suitable for X-ray structure analysis were obtained after six days by the slow evaporation of the above solution in air.

## Refinement

H atoms were treated as riding atoms with N—H, 0.86Å, C—H(aromatic), 0.95 Å, with $U_{iso}$ = 1.2Ueq(C) allowed to ride. The H atoms attached to the water molecule were refined as riding atoms at positions deteremined from a difference Fourier with $U_{iso}$ = 1.5Ueq(O). An examination of a difference Fourier along the line of the N1 to N3 vector showed an elongated density peak. This was found to be best modelled as two half-hydrogen atoms attached to N1 and N3. All H atom positions were checked on a final difference Fourier.

The disordered trifluoromethyl group was modelled over two sites with restrained bonds and angles based on the average values found for the non-disordered trifluoromethyl group in the other molecule. The site occupancies were refined and restraints were applied to the thermal parameters. The terafluoroborate anion is also modelled as being disordered over two sites. The site occupancies were refined and restraints were applied to the bonds, angles and the thermal parameters.

### Computing details

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear* (Rigaku, 2005); data reduction: *CrystalClear* (Rigaku, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

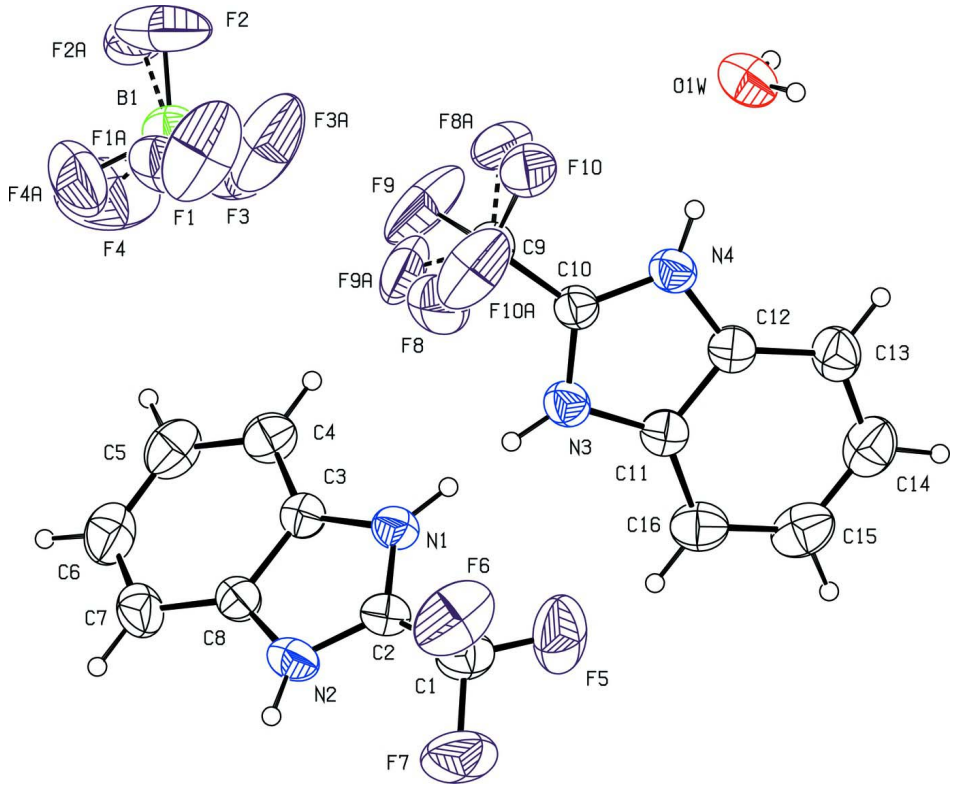


**Figure 1**

The molecular structure of the title compound, showing the atomic numbering scheme with 30% probability displacement ellipsoids. Both half hydrogens attached to N1 and N3 are included.

### 2-Trifluoromethyl-1*H*-benzimidazol-3-ium tetrafluoroborate– 2-trifluoromethyl-1*H*-benzimidazole–water (1/1/1)

*Crystal data*

$C_8H_6F_3N_2^+\cdot BF_4^-\cdot C_8H_5F_3N_2\cdot H_2O$
$M_r = 478.11$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
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$c = 11.458\ (2)$ Å
$\alpha = 92.48\ (3)°$
$\beta = 96.59\ (3)°$
$\gamma = 113.34\ (3)°$
$V = 1000.8\ (3)$ Å$^3$
$Z = 2$
$F(000) = 480$
$D_x = 1.587$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\theta = 0–25°$
$\mu = 0.17$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.36 × 0.32 × 0.28 mm

*Data collection*

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
CCD_Profile_fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.566, $T_{max}$ = 0.640

10445 measured reflections
4581 independent reflections
2280 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 3.0°
$h$ = −11→11
$k$ = −14→14
$l$ = −14→14

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.195
$S$ = 1.03
4581 reflections
355 parameters
65 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
$w = 1/[\sigma^2(F_o^2) + (0.073P)^2 + 0.2894P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.020 (4)

*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 of $F^2$ against ALL reflections. The weighted R-factor wR and goodness 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 threshold expression of $F^2 > 2$sigma($F^2$) is used only for calculating R-factors(gt) 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| F5 | −0.1135 (3) | 0.6112 (3) | 0.9237 (2) | 0.1358 (10) | |
| F6 | 0.0425 (3) | 0.6539 (3) | 1.0868 (3) | 0.1405 (11) | |
| F7 | −0.1136 (3) | 0.7537 (3) | 1.0522 (3) | 0.1382 (10) | |
| N1 | 0.1904 (3) | 0.7918 (2) | 0.8667 (2) | 0.0594 (6) | |
| H1 | 0.1676 | 0.7165 | 0.8274 | 0.071* | 0.50 |
| N2 | 0.1829 (3) | 0.9413 (3) | 0.9962 (2) | 0.0671 (7) | |
| H2A | 0.1531 | 0.9753 | 1.0539 | 0.081* | |
| C1 | −0.0170 (5) | 0.7072 (4) | 1.0035 (3) | 0.0815 (10) | |
| C2 | 0.1171 (4) | 0.8130 (3) | 0.9543 (2) | 0.0593 (7) | |
| C3 | 0.3121 (3) | 0.9151 (3) | 0.8501 (2) | 0.0562 (7) | |
| C4 | 0.4274 (4) | 0.9514 (3) | 0.7713 (3) | 0.0740 (9) | |
| H4 | 0.4338 | 0.8885 | 0.7171 | 0.089* | |
| C5 | 0.5317 (5) | 1.0842 (4) | 0.7770 (3) | 0.0882 (11) | |
| H5 | 0.6102 | 1.1119 | 0.7251 | 0.106* | |
| C6 | 0.5231 (5) | 1.1781 (4) | 0.8579 (4) | 0.0926 (12) | |

| | | | | | |
|---|---|---|---|---|---|
| H6 | 0.5951 | 1.2674 | 0.8580 | 0.111* | |
| C7 | 0.4121 (4) | 1.1439 (3) | 0.9378 (4) | 0.0810 (10) | |
| H7 | 0.4078 | 1.2068 | 0.9931 | 0.097* | |
| C8 | 0.3070 (4) | 1.0102 (3) | 0.9311 (2) | 0.0587 (7) | |
| N3 | 0.1071 (3) | 0.5575 (2) | 0.7327 (2) | 0.0622 (6) | |
| H3 | 0.1364 | 0.6341 | 0.7717 | 0.075* | 0.50 |
| N4 | 0.1163 (3) | 0.3728 (2) | 0.6582 (2) | 0.0627 (6) | |
| H4A | 0.1544 | 0.3135 | 0.6429 | 0.075* | |
| C9 | 0.3685 (3) | 0.5281 (2) | 0.7895 (2) | 0.0757 (9) | |
| C10 | 0.1977 (3) | 0.4870 (3) | 0.7266 (2) | 0.0569 (7) | |
| F8 | 0.3784 (12) | 0.5766 (11) | 0.8977 (4) | 0.130 (4) | 0.518 (14) |
| F9 | 0.4883 (7) | 0.6155 (10) | 0.7417 (9) | 0.163 (5) | 0.518 (14) |
| F10 | 0.4064 (9) | 0.4244 (5) | 0.8009 (8) | 0.105 (3) | 0.518 (14) |
| F8A | 0.4595 (8) | 0.4758 (11) | 0.7415 (10) | 0.161 (5) | 0.482 (14) |
| F9A | 0.4470 (9) | 0.6579 (3) | 0.7890 (10) | 0.117 (3) | 0.482 (14) |
| F10A | 0.3750 (11) | 0.5061 (12) | 0.9007 (4) | 0.135 (4) | 0.482 (14) |
| C11 | −0.0450 (4) | 0.4836 (3) | 0.6635 (2) | 0.0593 (7) | |
| C12 | −0.0405 (4) | 0.3665 (3) | 0.6161 (2) | 0.0602 (7) | |
| C13 | −0.1752 (4) | 0.2705 (3) | 0.5431 (3) | 0.0771 (9) | |
| H13 | −0.1705 | 0.1930 | 0.5106 | 0.093* | |
| C14 | −0.3154 (5) | 0.2961 (4) | 0.5213 (3) | 0.0897 (11) | |
| H14 | −0.4098 | 0.2332 | 0.4743 | 0.108* | |
| C15 | −0.3204 (5) | 0.4133 (5) | 0.5675 (3) | 0.0921 (11) | |
| H15 | −0.4180 | 0.4270 | 0.5492 | 0.110* | |
| C16 | −0.1879 (5) | 0.5100 (4) | 0.6388 (3) | 0.0786 (9) | |
| H16 | −0.1926 | 0.5884 | 0.6690 | 0.094* | |
| F1 | 0.8155 (16) | 0.8437 (14) | 0.8026 (9) | 0.191 (5) | 0.507 (14) |
| F2 | 0.9801 (12) | 0.8884 (13) | 0.6676 (9) | 0.164 (5) | 0.507 (14) |
| F3 | 0.7345 (11) | 0.8971 (12) | 0.6305 (8) | 0.131 (3) | 0.507 (14) |
| F4 | 0.9301 (13) | 1.0476 (8) | 0.7603 (10) | 0.175 (4) | 0.507 (14) |
| F1A | 0.8505 (12) | 0.8938 (8) | 0.8232 (5) | 0.105 (3) | 0.493 (14) |
| F2A | 1.0041 (11) | 0.9229 (11) | 0.6739 (11) | 0.123 (3) | 0.493 (14) |
| F3A | 0.7326 (12) | 0.8392 (17) | 0.6363 (9) | 0.208 (6) | 0.493 (14) |
| F4A | 0.875 (2) | 1.0469 (10) | 0.7068 (16) | 0.233 (6) | 0.493 (14) |
| B1 | 0.8652 (5) | 0.9202 (4) | 0.7116 (3) | 0.0835 (11) | |
| O1W | 0.2248 (3) | 0.1817 (2) | 0.6036 (2) | 0.0972 (8) | |
| H1A | 0.2132 | 0.1781 | 0.5299 | 0.146* | |
| H1B | 0.1572 | 0.1131 | 0.6279 | 0.146* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F5 | 0.121 (2) | 0.1109 (18) | 0.1217 (19) | −0.0148 (15) | 0.0434 (16) | 0.0023 (15) |
| F6 | 0.122 (2) | 0.165 (2) | 0.150 (2) | 0.0578 (18) | 0.0486 (17) | 0.103 (2) |
| F7 | 0.125 (2) | 0.139 (2) | 0.180 (3) | 0.0620 (17) | 0.098 (2) | 0.0385 (19) |
| N1 | 0.0647 (15) | 0.0599 (15) | 0.0577 (14) | 0.0281 (12) | 0.0147 (11) | 0.0044 (11) |
| N2 | 0.0804 (17) | 0.0739 (17) | 0.0576 (14) | 0.0435 (15) | 0.0091 (13) | −0.0042 (13) |
| C1 | 0.081 (2) | 0.090 (3) | 0.085 (2) | 0.039 (2) | 0.032 (2) | 0.021 (2) |
| C2 | 0.0667 (18) | 0.0633 (19) | 0.0581 (17) | 0.0347 (15) | 0.0152 (14) | 0.0105 (14) |
| C3 | 0.0581 (17) | 0.0588 (17) | 0.0529 (16) | 0.0254 (14) | 0.0055 (13) | 0.0079 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C4 | 0.074 (2) | 0.083 (2) | 0.0670 (19) | 0.0312 (19) | 0.0200 (16) | 0.0147 (17) |
| C5 | 0.076 (2) | 0.093 (3) | 0.093 (3) | 0.026 (2) | 0.0198 (19) | 0.035 (2) |
| C6 | 0.077 (2) | 0.067 (2) | 0.126 (3) | 0.0241 (19) | −0.003 (2) | 0.028 (2) |
| C7 | 0.078 (2) | 0.059 (2) | 0.103 (3) | 0.0329 (18) | −0.015 (2) | −0.0030 (18) |
| C8 | 0.0611 (17) | 0.0600 (18) | 0.0571 (16) | 0.0299 (15) | −0.0016 (14) | 0.0015 (14) |
| N3 | 0.0662 (15) | 0.0575 (14) | 0.0627 (14) | 0.0228 (13) | 0.0174 (12) | 0.0043 (11) |
| N4 | 0.0675 (16) | 0.0614 (15) | 0.0619 (14) | 0.0271 (12) | 0.0180 (12) | 0.0018 (12) |
| C9 | 0.066 (2) | 0.071 (2) | 0.084 (2) | 0.0213 (18) | 0.0118 (18) | −0.0024 (19) |
| C10 | 0.0589 (17) | 0.0561 (17) | 0.0551 (16) | 0.0210 (14) | 0.0150 (13) | 0.0039 (13) |
| F8 | 0.117 (5) | 0.162 (7) | 0.106 (5) | 0.075 (6) | −0.042 (4) | −0.067 (4) |
| F9 | 0.061 (3) | 0.191 (8) | 0.237 (10) | 0.033 (5) | 0.047 (5) | 0.130 (8) |
| F10 | 0.078 (4) | 0.092 (3) | 0.151 (6) | 0.050 (3) | −0.013 (3) | −0.003 (3) |
| F8A | 0.065 (4) | 0.194 (10) | 0.207 (10) | 0.049 (6) | 0.009 (5) | −0.090 (8) |
| F9A | 0.053 (4) | 0.098 (4) | 0.168 (7) | 0.000 (3) | 0.001 (3) | 0.018 (4) |
| F10A | 0.088 (4) | 0.198 (9) | 0.100 (5) | 0.033 (6) | 0.008 (4) | 0.068 (5) |
| C11 | 0.0651 (18) | 0.0645 (18) | 0.0503 (15) | 0.0260 (15) | 0.0143 (14) | 0.0116 (13) |
| C12 | 0.0653 (19) | 0.0672 (19) | 0.0472 (15) | 0.0237 (15) | 0.0153 (14) | 0.0080 (13) |
| C13 | 0.080 (2) | 0.082 (2) | 0.0578 (18) | 0.0223 (18) | 0.0085 (16) | −0.0049 (16) |
| C14 | 0.078 (2) | 0.114 (3) | 0.062 (2) | 0.025 (2) | 0.0044 (17) | 0.002 (2) |
| C15 | 0.081 (3) | 0.135 (4) | 0.070 (2) | 0.054 (3) | 0.0062 (19) | 0.017 (2) |
| C16 | 0.085 (2) | 0.091 (2) | 0.072 (2) | 0.048 (2) | 0.0146 (19) | 0.0147 (18) |
| F1 | 0.141 (6) | 0.243 (10) | 0.136 (7) | 0.019 (8) | 0.012 (5) | 0.086 (8) |
| F2 | 0.181 (8) | 0.289 (13) | 0.104 (6) | 0.188 (10) | 0.009 (5) | −0.012 (6) |
| F3 | 0.102 (5) | 0.214 (8) | 0.092 (4) | 0.093 (5) | −0.016 (4) | −0.020 (4) |
| F4 | 0.173 (7) | 0.131 (6) | 0.174 (8) | 0.018 (5) | 0.037 (6) | −0.071 (5) |
| F1A | 0.134 (6) | 0.129 (5) | 0.060 (3) | 0.063 (5) | 0.018 (3) | −0.015 (3) |
| F2A | 0.091 (4) | 0.140 (6) | 0.143 (8) | 0.039 (4) | 0.053 (5) | 0.031 (5) |
| F3A | 0.106 (5) | 0.339 (14) | 0.083 (4) | −0.008 (7) | 0.013 (4) | −0.018 (7) |
| F4A | 0.264 (14) | 0.170 (7) | 0.361 (18) | 0.151 (8) | 0.140 (12) | 0.133 (9) |
| B1 | 0.087 (3) | 0.095 (3) | 0.076 (3) | 0.043 (3) | 0.015 (2) | 0.010 (2) |
| O1W | 0.117 (2) | 0.0938 (18) | 0.0889 (17) | 0.0516 (15) | 0.0183 (15) | −0.0090 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| F5—C1 | 1.301 (4) | C9—F8A | 1.306 (2) |
| F6—C1 | 1.305 (4) | C9—F10A | 1.306 (2) |
| F7—C1 | 1.311 (4) | C9—F8 | 1.307 (2) |
| N1—C2 | 1.312 (3) | C9—F10 | 1.311 (2) |
| N1—C3 | 1.388 (4) | C9—F9A | 1.312 (2) |
| N1—H1 | 0.8600 | C9—C10 | 1.471 (3) |
| N2—C2 | 1.331 (3) | C11—C12 | 1.388 (4) |
| N2—C8 | 1.378 (4) | C11—C16 | 1.398 (4) |
| N2—H2A | 0.8600 | C12—C13 | 1.384 (4) |
| C1—C2 | 1.475 (5) | C13—C14 | 1.367 (5) |
| C3—C8 | 1.382 (4) | C13—H13 | 0.9300 |
| C3—C4 | 1.387 (4) | C14—C15 | 1.386 (5) |
| C4—C5 | 1.371 (5) | C14—H14 | 0.9300 |
| C4—H4 | 0.9300 | C15—C16 | 1.369 (5) |
| C5—C6 | 1.385 (5) | C15—H15 | 0.9300 |
| C5—H5 | 0.9300 | C16—H16 | 0.9300 |

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|---|---|---|---|
| C6—C7 | 1.370 (5) | F1—B1 | 1.368 (7) |
| C6—H6 | 0.9300 | F2—B1 | 1.332 (6) |
| C7—C8 | 1.379 (4) | F3—B1 | 1.324 (7) |
| C7—H7 | 0.9300 | F4—B1 | 1.346 (7) |
| N3—C10 | 1.316 (3) | F1A—B1 | 1.332 (7) |
| N3—C11 | 1.383 (4) | F2A—B1 | 1.332 (7) |
| N3—H3 | 0.8600 | F3A—B1 | 1.332 (7) |
| N4—C10 | 1.329 (3) | F4A—B1 | 1.361 (7) |
| N4—C12 | 1.380 (4) | O1W—H1A | 0.8362 |
| N4—H4A | 0.8600 | O1W—H1B | 0.8349 |
| C9—F9 | 1.305 (2) | | |

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|---|---|---|---|
| C2—N1—C3 | 106.4 (2) | F8A—C9—F9A | 106.1 (3) |
| C2—N1—H1 | 126.8 | F10A—C9—F9A | 105.4 (3) |
| C3—N1—H1 | 126.8 | F9—C9—C10 | 116.2 (4) |
| C2—N2—C8 | 108.2 (2) | F8A—C9—C10 | 114.7 (4) |
| C2—N2—H2A | 125.9 | F10A—C9—C10 | 114.2 (5) |
| C8—N2—H2A | 125.9 | F8—C9—C10 | 110.4 (4) |
| F5—C1—F6 | 107.6 (3) | F10—C9—C10 | 110.7 (3) |
| F5—C1—F7 | 106.9 (3) | F9A—C9—C10 | 108.2 (4) |
| F6—C1—F7 | 105.5 (3) | N3—C10—N4 | 112.2 (2) |
| F5—C1—C2 | 112.5 (3) | N3—C10—C9 | 124.2 (2) |
| F6—C1—C2 | 112.1 (3) | N4—C10—C9 | 123.6 (2) |
| F7—C1—C2 | 111.8 (3) | N3—C11—C12 | 108.4 (3) |
| N1—C2—N2 | 111.6 (3) | N3—C11—C16 | 130.7 (3) |
| N1—C2—C1 | 124.3 (3) | C12—C11—C16 | 120.9 (3) |
| N2—C2—C1 | 124.0 (3) | N4—C12—C13 | 132.0 (3) |
| C8—C3—C4 | 120.4 (3) | N4—C12—C11 | 105.6 (2) |
| C8—C3—N1 | 108.3 (2) | C13—C12—C11 | 122.3 (3) |
| C4—C3—N1 | 131.3 (3) | C14—C13—C12 | 116.3 (3) |
| C5—C4—C3 | 117.0 (3) | C14—C13—H13 | 121.8 |
| C5—C4—H4 | 121.5 | C12—C13—H13 | 121.8 |
| C3—C4—H4 | 121.5 | C13—C14—C15 | 121.6 (3) |
| C4—C5—C6 | 121.7 (3) | C13—C14—H14 | 119.2 |
| C4—C5—H5 | 119.2 | C15—C14—H14 | 119.2 |
| C6—C5—H5 | 119.2 | C16—C15—C14 | 122.9 (4) |
| C7—C6—C5 | 122.2 (3) | C16—C15—H15 | 118.6 |
| C7—C6—H6 | 118.9 | C14—C15—H15 | 118.6 |
| C5—C6—H6 | 118.9 | C15—C16—C11 | 115.9 (3) |
| C6—C7—C8 | 115.8 (3) | C15—C16—H16 | 122.0 |
| C6—C7—H7 | 122.1 | C11—C16—H16 | 122.0 |
| C8—C7—H7 | 122.1 | F3—B1—F2 | 111.2 (6) |
| N2—C8—C7 | 131.5 (3) | F2A—B1—F3A | 109.3 (8) |
| N2—C8—C3 | 105.5 (2) | F2A—B1—F1A | 115.8 (7) |
| C7—C8—C3 | 123.0 (3) | F3A—B1—F1A | 112.5 (7) |
| C10—N3—C11 | 106.1 (2) | F3—B1—F4 | 110.9 (6) |
| C10—N3—H3 | 126.9 | F2—B1—F4 | 111.7 (7) |
| C11—N3—H3 | 126.9 | F1A—B1—F4 | 82.7 (7) |
| C10—N4—C12 | 107.6 (2) | F2A—B1—F4A | 105.0 (7) |

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|---|---|---|---|
| C10—N4—H4A | 126.2 | F3A—B1—F4A | 107.9 (8) |
| C12—N4—H4A | 126.2 | F1A—B1—F4A | 105.7 (7) |
| F8A—C9—F10A | 107.6 (4) | F3—B1—F1 | 109.8 (7) |
| F9—C9—F8 | 107.6 (4) | F2—B1—F1 | 107.6 (7) |
| F9—C9—F10 | 106.5 (3) | F4—B1—F1 | 105.4 (6) |
| F8—C9—F10 | 104.6 (3) | H1A—O1W—H1B | 112.4 |
| | | | |
| C3—N1—C2—N2 | −0.3 (3) | C12—N4—C10—C9 | 178.8 (2) |
| C3—N1—C2—C1 | −178.0 (3) | F9—C9—C10—N3 | −79.8 (7) |
| C8—N2—C2—N1 | 0.8 (3) | F8A—C9—C10—N3 | −155.5 (8) |
| C8—N2—C2—C1 | 178.5 (3) | F10A—C9—C10—N3 | 79.6 (7) |
| F5—C1—C2—N1 | −33.5 (5) | F8—C9—C10—N3 | 43.1 (6) |
| F6—C1—C2—N1 | 87.9 (4) | F10—C9—C10—N3 | 158.5 (5) |
| F7—C1—C2—N1 | −153.8 (3) | F9A—C9—C10—N3 | −37.4 (6) |
| F5—C1—C2—N2 | 149.1 (3) | F9—C9—C10—N4 | 101.1 (7) |
| F6—C1—C2—N2 | −89.5 (4) | F8A—C9—C10—N4 | 25.4 (8) |
| F7—C1—C2—N2 | 28.8 (5) | F10A—C9—C10—N4 | −99.4 (7) |
| C2—N1—C3—C8 | −0.3 (3) | F8—C9—C10—N4 | −135.9 (6) |
| C2—N1—C3—C4 | 179.1 (3) | F10—C9—C10—N4 | −20.6 (6) |
| C8—C3—C4—C5 | −1.1 (4) | F9A—C9—C10—N4 | 143.6 (6) |
| N1—C3—C4—C5 | 179.6 (3) | C10—N3—C11—C12 | −0.1 (3) |
| C3—C4—C5—C6 | 0.3 (5) | C10—N3—C11—C16 | 179.6 (3) |
| C4—C5—C6—C7 | 0.9 (6) | C10—N4—C12—C13 | −179.4 (3) |
| C5—C6—C7—C8 | −1.2 (5) | C10—N4—C12—C11 | 0.3 (3) |
| C2—N2—C8—C7 | 179.7 (3) | N3—C11—C12—N4 | −0.1 (3) |
| C2—N2—C8—C3 | −0.9 (3) | C16—C11—C12—N4 | −179.8 (3) |
| C6—C7—C8—N2 | 179.8 (3) | N3—C11—C12—C13 | 179.6 (3) |
| C6—C7—C8—C3 | 0.4 (4) | C16—C11—C12—C13 | −0.2 (4) |
| C4—C3—C8—N2 | −178.8 (3) | N4—C12—C13—C14 | 178.5 (3) |
| N1—C3—C8—N2 | 0.7 (3) | C11—C12—C13—C14 | −1.1 (4) |
| C4—C3—C8—C7 | 0.7 (4) | C12—C13—C14—C15 | 1.6 (5) |
| N1—C3—C8—C7 | −179.8 (3) | C13—C14—C15—C16 | −1.0 (6) |
| C11—N3—C10—N4 | 0.3 (3) | C14—C15—C16—C11 | −0.3 (5) |
| C11—N3—C10—C9 | −178.8 (2) | N3—C11—C16—C15 | −178.9 (3) |
| C12—N4—C10—N3 | −0.4 (3) | C12—C11—C16—C15 | 0.8 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N4—H4*A*···O1*W* | 0.86 | 1.84 | 2.698 (3) | 177 |
| N1—H1···N3 | 0.86 | 1.86 | 2.718 (3) | 175 |
| N3—H3···N1 | 0.86 | 1.86 | 2.718 (3) | 175 |