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# 2-Trifluoromethyl-1*H*-benzimidazole

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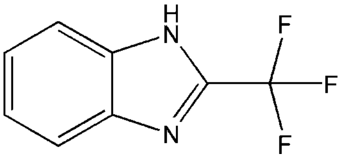
Key indicators: single-crystal X-ray study; *T* = 293 K; mean $\sigma$(C–C) = 0.005 Å; disorder in main residue; *R* factor = 0.071; *wR* factor = 0.168; data-to-parameter ratio = 11.8.

The asymmetric unit of the title compound, $C_8H_5F_3N_2$, consists of two half-molecules, one lies on a mirror plane and the other is generated by twofold rotation symmetry, with the axis running through the trifluoromethyl C atom and the attached benzimidazole C atom. The two 2-trifluoromethyl-1*H*-benzimidazole molecules are connected by N—H⋯N hydrogen bonds involving the disordered NH H atoms into chains running parallel to the *c* axis. One of the trifluoromethyl groups is disordered over two orientations of equal occupancy.

## Related literature

For background to ferroelectric complexes, see: Fu *et al.* (2011); Zhang *et al.* (2010). For related structures, see: Liu (2011*a*,*b*, 2012*a*,*b*,*c*). For graph-set analysis, see: Bernstein *et al.* (1995).



## Experimental

### *Crystal data*

$C_8H_5F_3N_2$
$M_r$ = 186.14
Orthorhombic, *Pbcm*
*a* = 11.859 (2) Å
*b* = 7.2154 (14) Å
*c* = 19.508 (4) Å
*V* = 1669.2 (5) Å$^3$
*Z* = 8
Mo *Kα* radiation
$\mu$ = 0.14 mm$^{-1}$
*T* = 293 K
0.36 × 0.32 × 0.28 mm

### *Data collection*

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{\min}$ = 0.952, $T_{\max}$ = 0.962
13301 measured reflections
1523 independent reflections
983 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.074

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.168
*S* = 1.04
1523 reflections
129 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.28 e Å$^{-3}$
$\Delta\rho_{\min}$ = −0.23 e Å$^{-3}$

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

| *D*—H⋯*A* | *D*—H | H⋯*A* | *D*⋯*A* | *D*—H⋯*A* |
|---|---|---|---|---|
| N1—H1*A*⋯N4 | 0.86 | 2.03 | 2.891 (3) | 173 |
| N4—H4*A*⋯N1 | 0.86 | 2.03 | 2.891 (3) | 174 |

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: *SHELXL97*.

The author thanks an anonymous advisor from the Ordered Matter Science Research Centre, Southeast University, for great help in the revision of this paper.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GO2052).

## References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
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*a*). *Acta Cryst.* E**68**, o342.
Liu, M.-L. (2012*b*). *Acta Cryst.* E**68**, o1012.
Liu, M.-L. (2012*c*). *Acta Cryst.* E**68**, o1076.
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

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## 2-Trifluoromethyl-1*H*-benzimidazole

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 potential ferroelectric 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 has an asymmetric unit that consists of two half 2-trifluoromethyl-1*H*-benzimidazole molecules (Fig 1). In each of these molecules the H atoms attached to the N atoms are shared 50/50 over both sites.

One of these molecule sits on a mirror plane at *c* = 0.75 and the other sits on a 2-fold axis at *b* = 0.25 and *c* = 0.5 with the axis running through atoms C1 and C2 of the trifluoromethyl group.

The molecules of, I, are hydrogen bonded together to form $C^2_3(8)$ chain,(Bernstein *et al.*, 1995), which run parallel to the c-axis. Half by N1···N4, N4···N1 and N1..N4 chains. and half by N4···N1, N1···N4 and N4···N1 chaims, (in each case the first atom is the donor and the second the acceptor).

One of the trifluoromethyl groups is disordered.

### Experimental

0.144 g (1 mmol) of 2-trifluoromethyl-1*H*-benzimidazole was dissolved in 30 ml of ethanol to give a solution at the ambient temperature. Single crystals suitable for X-ray structure analysis were obtained by the slow evaporation of the above solution after 3 days in air.

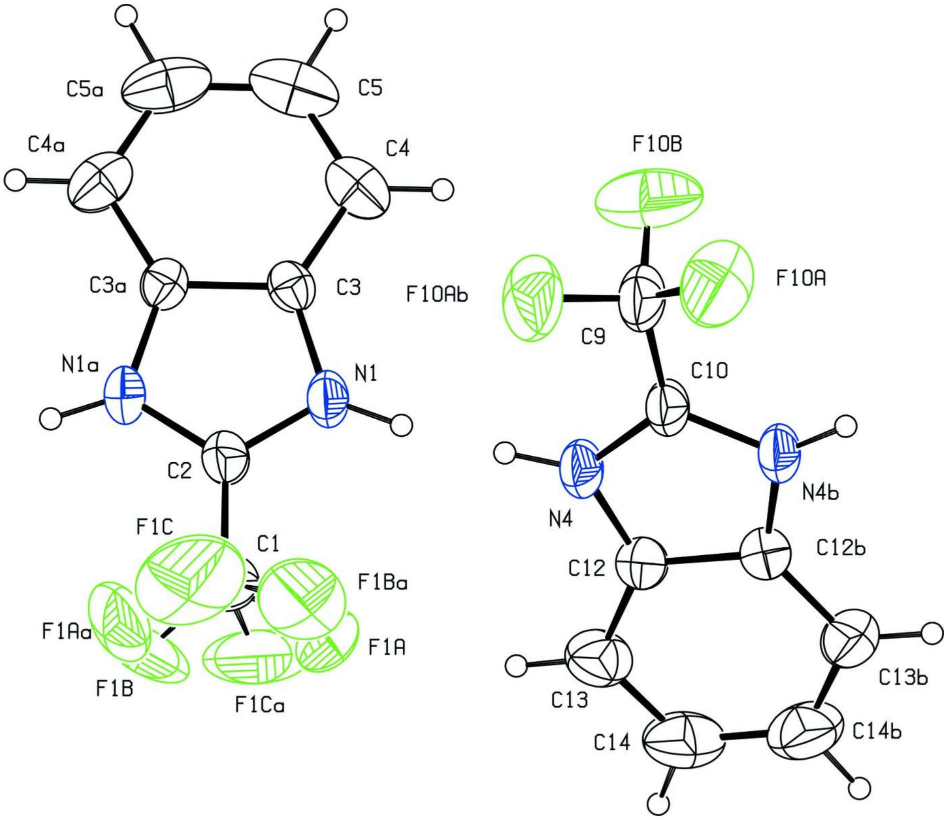
### Refinement

H atoms were treated as riding atoms with N—H, 0.86Å, C—H(aromatic), 0.95 Å, with $U_{\rm iso}$ = 1.2Ueq(C) allowed to ride. An examination of a difference map along the line of the N1 to N2 vector showed an elongated density peak. This was found to be best modelled as two half-hydrogen atoms attached to N1 and N4. These positions were checked on the final difference map.

The disordered trifluoromethyl was modelled with restrained bonds and angles based on the average values found for the non-disordered trifluoromethyl group with initial positions being derived from a difference map. The action of the symmetry axis passing molecule produced a set of six F atoms spaced around a regular hexagon. Each of these F atoms was given a site occupancy of 0.5. In the final stages of refinement the group was refined as a riding and rotating group as for a methyl group. This model is not perfect and as a result there are several C Alerts.

## 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: *SHELXL97* (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 N2 and the disordered fluorine atoms are included.

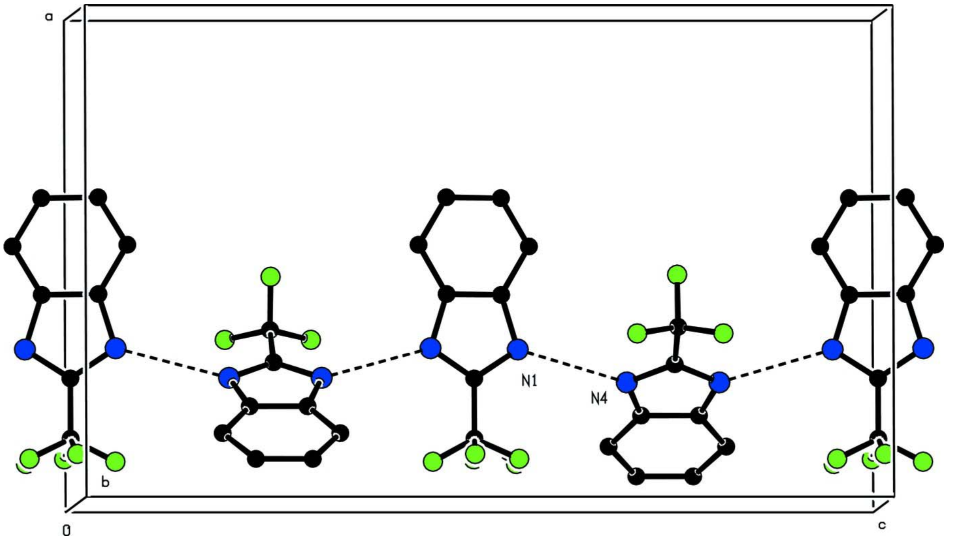


**Figure 2**

View of the C3 chain running parallel to the c-axis. For clarity all hydrogen atoms are omitted.

## 2-Trifluoromethyl-1*H*-benzimidazole

*Crystal data*

$C_8H_5F_3N_2$
$M_r = 186.14$
Orthorhombic, *Pbcm*
Hall symbol: -P 2c 2b
$a = 11.859\ (2)$ Å
$b = 7.2154\ (14)$ Å
$c = 19.508\ (4)$ Å
$V = 1669.2\ (5)$ Å$^3$
$Z = 8$

$F(000) = 752$
$D_x = 1.481$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\theta = 0–25°$
$\mu = 0.14$ 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)
$T_{\min} = 0.952$, $T_{\max} = 0.962$

13301 measured reflections
1523 independent reflections
983 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.074$
$\theta_{\max} = 25.0°$, $\theta_{\min} = 3.3°$
$h = -14 \rightarrow 14$
$k = -8 \rightarrow 8$
$l = -23 \rightarrow 22$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.071$
$wR(F^2) = 0.168$
$S = 1.04$
1523 reflections
129 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
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 1.2173P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.28$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.23$ e Å$^{-3}$

*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 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 $F^2 > 2\mathrm{sigma}(F^2)$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{\mathrm{iso}}$*/$U_{\mathrm{eq}}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C2 | 0.2645 (4) | 0.2500 | 0.5000 | 0.0595 (12) | |
| C1 | 0.14185 (18) | 0.2500 | 0.5000 | 0.101 (2) | |
| F1A | 0.09271 (18) | 0.1770 | 0.5534 | 0.157 (4) | 0.50 |
| F1B | 0.09835 (18) | 0.1655 | 0.4469 | 0.191 (5) | 0.50 |
| F1C | 0.10542 (18) | 0.4210 | 0.4964 | 0.213 (5) | 0.50 |
| N1 | 0.3246 (2) | 0.2091 (3) | 0.55507 (11) | 0.0576 (7) | |
| H1A | 0.3000 | 0.1795 | 0.5951 | 0.069* | 0.50 |
| C3 | 0.4353 (2) | 0.2242 (4) | 0.53443 (14) | 0.0495 (7) | |
| C4 | 0.5347 (3) | 0.1964 (5) | 0.5697 (2) | 0.0760 (11) | |
| H4 | 0.5350 | 0.1606 | 0.6155 | 0.091* | |
| C5 | 0.6321 (3) | 0.2236 (6) | 0.5345 (2) | 0.0986 (16) | |
| H5 | 0.7006 | 0.2067 | 0.5568 | 0.118* | |
| F10A | 0.3495 (3) | 0.4573 (4) | 0.80332 (12) | 0.1403 (12) | |
| F10B | 0.4734 (4) | 0.3146 (6) | 0.7500 | 0.1557 (19) | |
| N4 | 0.2610 (2) | 0.1033 (4) | 0.69268 (12) | 0.0641 (8) | |
| H4A | 0.2749 | 0.1364 | 0.6512 | 0.077* | 0.50 |
| C9 | 0.3662 (6) | 0.3519 (8) | 0.7500 | 0.0806 (17) | |
| C10 | 0.2953 (4) | 0.1861 (6) | 0.7500 | 0.0605 (12) | |
| C12 | 0.1984 (3) | −0.0467 (5) | 0.71420 (15) | 0.0623 (9) | |
| C13 | 0.1394 (3) | −0.1800 (6) | 0.6772 (2) | 0.0855 (12) | |
| H13 | 0.1382 | −0.1800 | 0.6295 | 0.103* | |
| C14 | 0.0830 (4) | −0.3113 (7) | 0.7148 (2) | 0.1073 (16) | |
| H14 | 0.0434 | −0.4036 | 0.6917 | 0.129* | |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C2 | 0.059 (3) | 0.076 (3) | 0.044 (3) | 0.000 | 0.000 | −0.002 (2) |
| C1 | 0.066 (4) | 0.134 (6) | 0.102 (5) | 0.000 | 0.000 | 0.004 (4) |
| F1A | 0.078 (4) | 0.304 (13) | 0.088 (5) | −0.044 (9) | 0.024 (5) | 0.041 (5) |
| F1B | 0.075 (5) | 0.376 (17) | 0.121 (6) | −0.035 (10) | −0.039 (5) | −0.054 (7) |
| F1C | 0.089 (5) | 0.263 (10) | 0.288 (12) | 0.077 (6) | 0.034 (12) | 0.078 (11) |
| N1 | 0.0703 (17) | 0.0672 (18) | 0.0354 (13) | −0.0017 (13) | −0.0008 (13) | 0.0038 (11) |
| C3 | 0.0575 (18) | 0.0449 (17) | 0.0461 (15) | 0.0004 (14) | −0.0057 (14) | −0.0042 (13) |
| C4 | 0.082 (3) | 0.062 (2) | 0.084 (2) | 0.0088 (19) | −0.026 (2) | −0.0089 (19) |
| C5 | 0.070 (2) | 0.068 (3) | 0.158 (5) | 0.011 (2) | −0.030 (2) | −0.033 (3) |
| F10A | 0.216 (3) | 0.113 (2) | 0.0923 (18) | −0.069 (2) | 0.0224 (18) | −0.0384 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| F10B | 0.097 (3) | 0.117 (3) | 0.252 (6) | −0.040 (3) | 0.000 | 0.000 |
| N4 | 0.081 (2) | 0.0755 (19) | 0.0357 (13) | −0.0105 (15) | 0.0007 (13) | −0.0028 (13) |
| C9 | 0.117 (5) | 0.082 (4) | 0.043 (3) | −0.027 (4) | 0.000 | 0.000 |
| C10 | 0.076 (3) | 0.069 (3) | 0.037 (2) | −0.010 (3) | 0.000 | 0.000 |
| C12 | 0.059 (2) | 0.073 (2) | 0.0549 (17) | −0.0047 (17) | 0.0013 (15) | −0.0026 (16) |
| C13 | 0.076 (3) | 0.098 (3) | 0.083 (3) | −0.012 (2) | −0.001 (2) | −0.025 (2) |
| C14 | 0.087 (3) | 0.099 (3) | 0.135 (4) | −0.030 (2) | −0.005 (2) | −0.022 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C2—N1$^{i}$ | 1.323 (3) | C5—H5 | 0.9300 |
| C2—N1 | 1.323 (3) | F10A—C9 | 1.303 (4) |
| C2—C1 | 1.454 (5) | F10B—C9 | 1.300 (7) |
| C1—F1A$^{i}$ | 1.3052 | N4—C10 | 1.331 (3) |
| C1—F1A | 1.3053 | N4—C12 | 1.378 (4) |
| C1—F1B | 1.3079 | N4—H4A | 0.8600 |
| C1—F1B$^{i}$ | 1.3079 | C9—F10A$^{ii}$ | 1.304 (4) |
| C1—F1C$^{i}$ | 1.3095 | C9—C10 | 1.462 (7) |
| C1—F1C | 1.3095 | C10—N4$^{ii}$ | 1.331 (3) |
| N1—C3 | 1.377 (4) | C12—C13 | 1.392 (5) |
| N1—H1A | 0.8600 | C12—C12$^{ii}$ | 1.397 (6) |
| C3—C4 | 1.380 (4) | C13—C14 | 1.372 (6) |
| C3—C3$^{i}$ | 1.394 (5) | C13—H13 | 0.9300 |
| C4—C5 | 1.359 (5) | C14—C14$^{ii}$ | 1.375 (9) |
| C4—H4 | 0.9300 | C14—H14 | 0.9300 |
| C5—C5$^{i}$ | 1.399 (9) | | |
| | | | |
| N1$^{i}$—C2—N1 | 114.7 (4) | C4—C5—C5$^{i}$ | 121.8 (2) |
| N1$^{i}$—C2—C1 | 122.6 (2) | C4—C5—H5 | 119.1 |
| N1—C2—C1 | 122.6 (2) | C5$^{i}$—C5—H5 | 119.1 |
| F1A—C1—F1B | 105.6 | C10—N4—C12 | 105.1 (3) |
| F1A$^{i}$—C1—F1B$^{i}$ | 105.6 | C10—N4—H4A | 127.4 |
| F1A$^{i}$—C1—F1C$^{i}$ | 106.0 | C12—N4—H4A | 127.4 |
| F1B$^{i}$—C1—F1C$^{i}$ | 105.4 | F10B—C9—F10A | 105.6 (4) |
| F1A—C1—F1C | 106.0 | F10B—C9—F10A$^{ii}$ | 105.6 (4) |
| F1B—C1—F1C | 105.4 | F10A—C9—F10A$^{ii}$ | 105.9 (5) |
| F1A$^{i}$—C1—C2 | 116.522 (6) | F10B—C9—C10 | 113.1 (5) |
| F1A—C1—C2 | 116.519 (5) | F10A—C9—C10 | 113.0 (3) |
| F1B—C1—C2 | 113.229 (5) | F10A$^{ii}$—C9—C10 | 113.0 (3) |
| F1B$^{i}$—C1—C2 | 113.230 (5) | N4—C10—N4$^{ii}$ | 114.3 (4) |
| F1C$^{i}$—C1—C2 | 109.263 (5) | N4—C10—C9 | 122.9 (2) |
| F1C—C1—C2 | 109.262 (5) | N4$^{ii}$—C10—C9 | 122.9 (2) |
| C2—N1—C3 | 105.0 (3) | N4—C12—C13 | 131.0 (3) |
| C2—N1—H1A | 127.5 | N4—C12—C12$^{ii}$ | 107.74 (16) |
| C3—N1—H1A | 127.5 | C13—C12—C12$^{ii}$ | 121.3 (2) |
| N1—C3—C4 | 131.0 (3) | C14—C13—C12 | 116.4 (4) |
| N1—C3—C3$^{i}$ | 107.64 (15) | C14—C13—H13 | 121.8 |
| C4—C3—C3$^{i}$ | 121.3 (2) | C12—C13—H13 | 121.8 |
| C5—C4—C3 | 116.9 (4) | C13—C14—C14$^{ii}$ | 122.3 (2) |
| C5—C4—H4 | 121.5 | C13—C14—H14 | 118.9 |

| | | | |
|---|---|---|---|
| C3—C4—H4 | 121.5 | C14$^{ii}$—C14—H14 | 118.9 |

| | | | |
|---|---|---|---|
| N1$^{i}$—C2—C1—F1A$^{i}$ | −11.43 (13) | N1—C3—C4—C5 | −179.7 (3) |
| N1—C2—C1—F1A$^{i}$ | 168.57 (13) | C3$^{i}$—C3—C4—C5 | 0.7 (5) |
| N1$^{i}$—C2—C1—F1A | 168.57 (13) | C3—C4—C5—C5$^{i}$ | −0.4 (7) |
| N1—C2—C1—F1A | −11.43 (13) | C12—N4—C10—N4$^{ii}$ | 0.2 (5) |
| N1$^{i}$—C2—C1—F1B | 45.84 (13) | C12—N4—C10—C9 | 179.2 (5) |
| N1—C2—C1—F1B | −134.16 (13) | F10B—C9—C10—N4 | −89.5 (4) |
| N1$^{i}$—C2—C1—F1B$^{i}$ | −134.16 (13) | F10A—C9—C10—N4 | 150.6 (4) |
| N1—C2—C1—F1B$^{i}$ | 45.84 (13) | F10A$^{ii}$—C9—C10—N4 | 30.4 (8) |
| N1$^{i}$—C2—C1—F1C$^{i}$ | 108.66 (13) | F10B—C9—C10—N4$^{ii}$ | 89.5 (4) |
| N1—C2—C1—F1C$^{i}$ | −71.34 (13) | F10A—C9—C10—N4$^{ii}$ | −30.4 (8) |
| N1$^{i}$—C2—C1—F1C | −71.34 (13) | F10A$^{ii}$—C9—C10—N4$^{ii}$ | −150.6 (4) |
| N1—C2—C1—F1C | 108.66 (13) | C10—N4—C12—C13 | 178.1 (4) |
| N1$^{i}$—C2—N1—C3 | −0.07 (14) | C10—N4—C12—C12$^{ii}$ | −0.1 (3) |
| C1—C2—N1—C3 | 179.93 (14) | N4—C12—C13—C14 | −178.8 (4) |
| C2—N1—C3—C4 | −179.4 (3) | C12$^{ii}$—C12—C13—C14 | −0.8 (4) |
| C2—N1—C3—C3$^{i}$ | 0.2 (3) | C12—C13—C14—C14$^{ii}$ | 0.8 (4) |

Symmetry codes: (i) *x*, −*y*+1/2, −*z*+1; (ii) *x*, *y*, −*z*+3/2.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···N4 | 0.86 | 2.03 | 2.891 (3) | 173 |
| N4—H4*A*···N1 | 0.86 | 2.03 | 2.891 (3) | 174 |