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# 3,3′-[1,2-Phenylenebis(methylene)]bis(1-ethyl-1*H*-benzimidazol-1-ium) bis(hexafluorophosphate)

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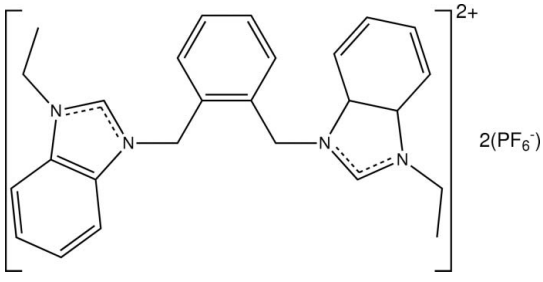
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; disorder in solvent or counterion; $R$ factor = 0.046; $wR$ factor = 0.098; data-to-parameter ratio = 18.1.

In the title compound, $C_{26}H_{28}N_4^{2+}\cdot 2PF_6^-$, the complete cation is generated by a crystallographic twofold axis. The benzimidazole ring is almost planar (r.m.s. deviation = 0.0207 Å) and makes dihedral angles of 50.12 (2)° with its symmetry-related component and 65.81 (2)° with the central benzene ring. In the crystal, molecules are linked into a three-dimensional network by C—H···F interactions. A $\pi$–$\pi$ interaction with a centroid–centroid distance of 3.530 (1) Å is observed. Four F atoms of the hexafluorophosphate anion are disordered over two sets of sites in a 0.889 (6):0.111 (6) ratio.

## Related literature

For the biological applications of benzimidazoles, see: Narasimhan *et al.* (2012). For a related structure, see: Haque *et al.* (2012).




## Experimental

### Crystal data

$C_{26}H_{28}N_4^{2+}\cdot 2PF_6^-$
$M_r$ = 686.46
Monoclinic, $C2/c$
$a$ = 23.2016 (5) Å
$b$ = 8.1526 (2) Å
$c$ = 16.9992 (4) Å
$\beta$ = 121.274 (1)°
$V$ = 2748.23 (11) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.27 mm$^{-1}$
$T$ = 100 K
0.26 × 0.26 × 0.14 mm

### Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.933, $T_{max}$ = 0.963
14787 measured reflections
3921 independent reflections
3156 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.037

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.098
$S$ = 1.05
3921 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 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···$A$ |
|---|---|---|---|---|
| C1—H1$A$···F6$^{i}$ | 0.95 | 2.42 | 3.142 (3) | 133 |
| C3—H3$A$···F5$^{ii}$ | 0.95 | 2.45 | 3.374 (2) | 166 |
| C5—H5$A$···F5$^{iii}$ | 0.95 | 2.52 | 3.420 (3) | 159 |
| C6—H6$A$···F4$^{iv}$ | 0.95 | 2.53 | 3.392 (2) | 151 |
| C8—H8$B$···F1$^{i}$ | 0.99 | 2.39 | 3.350 (3) | 164 |
| C13—H13$C$···F1$^{v}$ | 0.98 | 2.55 | 3.523 (2) | 174 |
| C13—H13$C$···F5$^{v}$ | 0.98 | 2.50 | 3.166 (2) | 125 |

Symmetry codes: (i) $x-1, y, z$; (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $x-\frac{1}{2}, y-\frac{1}{2}, z$; (iv) $-x+1, y, -z+\frac{3}{2}$; (v) $-x+1, -y+2, -z+2$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6760).

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

‡ Thomson Reuters ResearcherID: A-3561-2009.

# supplementary materials

*Acta Cryst.* (2012). E**68**, o1635 [doi:10.1107/S1600536812019344]

## 3,3′-[1,2-Phenylenebis(methylene)]bis(1-ethyl-1*H*-benzimidazol-1-ium) bis-(hexaflourophosphate)

**Rosenani A. Haque, Muhammad Adnan Iqbal, Mohd Mustaqim Rosli and Hoong-Kun Fun**

### Comment

Benzimidazole-constituted compounds are known as bioactive heterocyclic compounds that are of wide interest for biological and clinical applications (Narasimhan *et al.*, 2012). As a part of our ongoing studies in this area (Haque *et al.*, 2012), we now describe the title compound.

All parameters in the title compound (Fig. 1) are within normal ranges. The complete molecule is generated by a crystallographic two-fold axis. The benzimidazole (N1—N2/C1—C7) ring is planar with the r.m.s 0.0207 Å. It makes a dihedral angle of 50.12 (2)° with its symmetrical component and 65.81 (2) Å with the central benzene ring (C9—C11/C9A—C11A). Four fluorine atoms (F1—F4) of the hexafluorophosphate cation are disordered over two positions with the final refined occupancies of 0.889 (6):0.111 (6).

In the crystal structure, (Fig. 2), the molecules are linked into a three-dimensional network through intermolecular C—H···F hydrogen bonds (Table 1). A $\pi$-$\pi$ interaction with centroid-centroid distance of 3.530 (1) Å is observed (*Cg*1 = C2—C7).

### Experimental

A mixture of benzimidazole (1.18 g, 10 mmol) and potassium hydroxide (1.18 g, 15 mmol) in 30 ml of DMSO was stirred at room temperature (27–28°C) for 30 min. Ethyl bromide (0.75 ml, 10 mmol) was added drop-wise into this consistently stirring mixture and it was further stirred for 2 h at same temperature, then poured into water (150 ml) and was extracted by chloroform (3 × 20 ml). The extract was filtered by five plies of filter papers with medium porosity to collect a crystal-clear solution which was evaporated under vacuum to get *N*-ethylbenzimidazole (I) as a thick yellowish fluid. Then, a mixture of I (0.73 g, 5 mmol) and 1,2- bis(bromomethyl)benzene (0.66 g, 2.5 mmol) in 1,4-dioxane (20 ml) was refluxed at 110°C for 12 h. The bromide salt of title compound appeared as beige-colored precipitates in a dark brown solution. The mixture was filtered and the precipitates were washed by fresh 1,4-dioxane (3 *x* 5 ml) and dried at room temperature for 24 h. The soft lumps so obtained were dissolved in methanol (30 ml) along with $KPF_6$ (1.84 g, 10 mmol) and stirred for 3 h at room temperature. The white solid that appeared was filtered, washed by fresh methanol followed by water. The compound was dried at room temperature (1.53 g, 89.5%). A saturated solution of $2.2PF_6$ dissolved in acetonitrile (1 ml) was prepared. The compound was dissolved in it and the solution was evaporated at room temperature to collect colourless blocks of the title compound.

### Refinement

All H atoms attached to C atoms were fixed geometrically and refined as riding with C—H = 0.95–0.99 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(*C*-methyl). A rotating group model was applied to the methyl group. Four fluorine atoms (F1—F4) of the hexafluorophosphate cation are disordered over two positions with the final refined occupancies of

0.889 (6):0.111 (6).The minor component was refined isotropically.

### Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

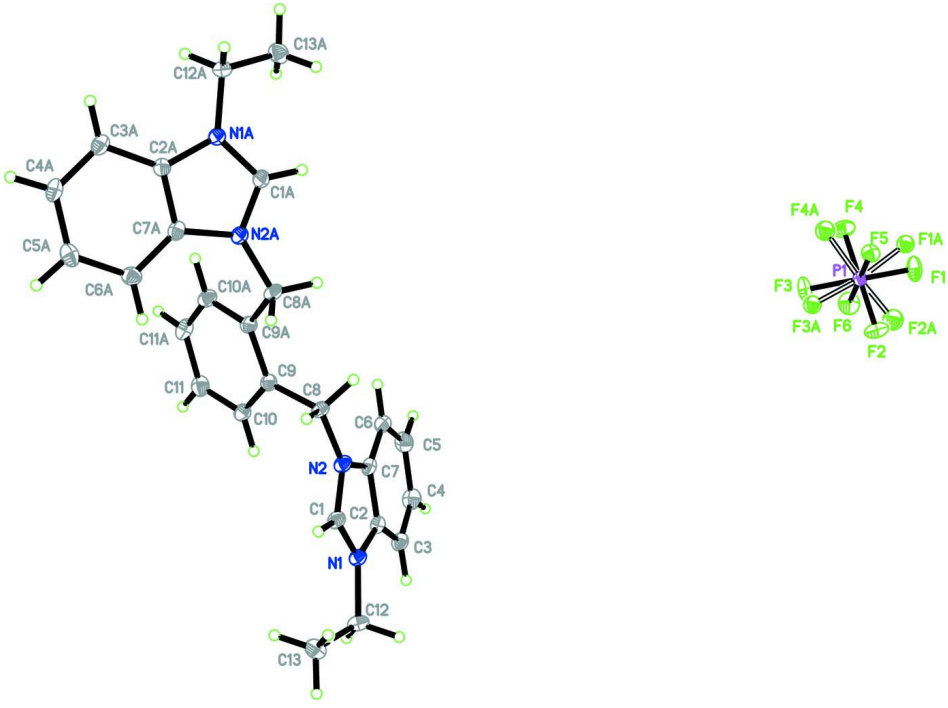


**Figure 1**

The molecular structure, showing 50% probability displacement ellipsoids. Hydrogen atoms are shown as spheres of arbitrary radius.

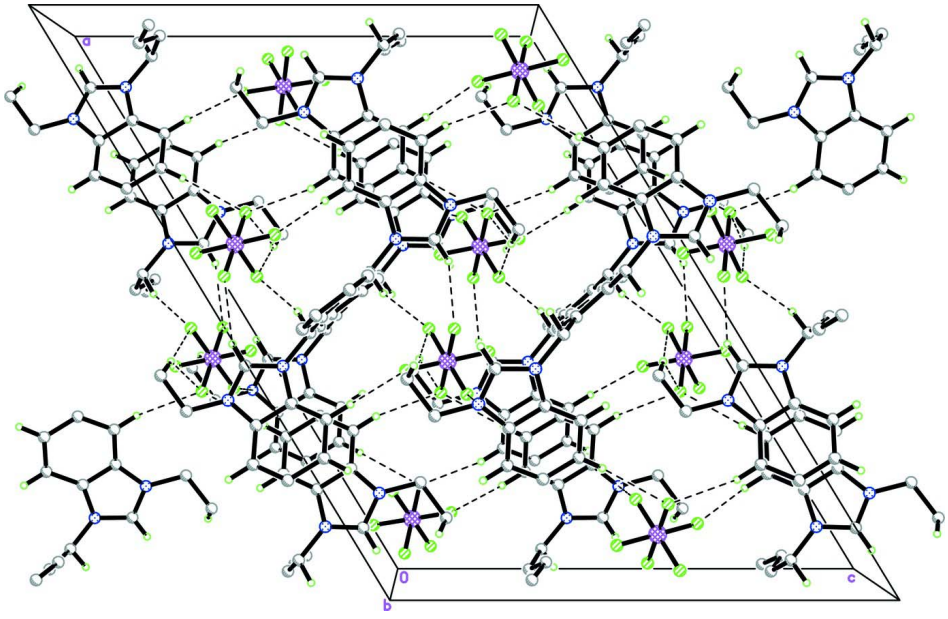

**Figure 2**

The crystal packing of (I). Dashed lines indicate hydrogen bonds. H atoms not involved in the hydrogen bond interactions have been omitted for clarity.

### 3,3′-[1,2-Phenylenebis(methylene)]bis(1-ethyl-1*H*-benzimidazol-1-ium) bis(hexaflourophosphate)

*Crystal data*

$C_{26}H_{28}N_4^{2+}\cdot 2PF_6^-$
$M_r = 686.46$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 23.2016\ (5)$ Å
$b = 8.1526\ (2)$ Å
$c = 16.9992\ (4)$ Å
$\beta = 121.274\ (1)°$
$V = 2748.23\ (11)$ Å$^3$
$Z = 4$
$F(000) = 1400$
$D_x = 1.659$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3899 reflections
$\theta = 2.5–29.7°$
$\mu = 0.27$ mm$^{-1}$
$T = 100$ K
Block, colourless
0.26 × 0.26 × 0.14 mm

*Data collection*

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.933$, $T_{max} = 0.963$
14787 measured reflections
3921 independent reflections
3156 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 29.8°$, $\theta_{min} = 2.1°$
$h = -32\rightarrow31$
$k = -11\rightarrow9$
$l = -23\rightarrow23$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.098$
$S = 1.05$
3921 reflections
217 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

| | |
|---|---|
| Secondary atom site location: difference Fourier map | $w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 4.2095P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| Hydrogen site location: inferred from neighbouring sites | $(\Delta/\sigma)_{max} = 0.001$ |
| H-atom parameters constrained | $\Delta\rho_{max} = 0.48$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.34$ e Å$^{-3}$ |

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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) |
|---|---|---|---|---|---|
| P1 | 0.89811 (2) | 0.80829 (6) | 0.89390 (3) | 0.01579 (11) | |
| F5 | 0.84112 (5) | 0.94532 (13) | 0.83897 (7) | 0.0220 (2) | |
| F6 | 0.95467 (6) | 0.67136 (15) | 0.94831 (8) | 0.0323 (3) | |
| F1 | 0.95400 (8) | 0.92423 (17) | 0.89472 (17) | 0.0309 (5) | 0.889 (6) |
| F2 | 0.91321 (10) | 0.8889 (2) | 0.98909 (10) | 0.0303 (5) | 0.889 (6) |
| F3 | 0.84260 (11) | 0.6929 (2) | 0.8940 (2) | 0.0311 (5) | 0.889 (6) |
| F4 | 0.88302 (12) | 0.7290 (2) | 0.79927 (10) | 0.0314 (5) | 0.889 (6) |
| F1A | 0.9350 (7) | 0.9043 (15) | 0.8457 (11) | 0.024 (3)* | 0.111 (6) |
| F2A | 0.9323 (8) | 0.9133 (18) | 0.9770 (10) | 0.032 (4)* | 0.111 (6) |
| F4A | 0.8573 (8) | 0.7032 (18) | 0.7950 (10) | 0.029 (3)* | 0.111 (6) |
| F3A | 0.8547 (9) | 0.713 (2) | 0.9237 (11) | 0.024 (4)* | 0.111 (6) |
| N1 | 0.16728 (7) | 0.66335 (17) | 1.09095 (9) | 0.0146 (3) | |
| N2 | 0.10920 (7) | 0.67626 (18) | 0.94040 (9) | 0.0154 (3) | |
| C1 | 0.10867 (8) | 0.7060 (2) | 1.01737 (11) | 0.0157 (3) | |
| H1A | 0.0717 | 0.7513 | 1.0192 | 0.019* | |
| C2 | 0.20844 (8) | 0.5997 (2) | 1.06084 (11) | 0.0142 (3) | |
| C3 | 0.27289 (8) | 0.5312 (2) | 1.10913 (12) | 0.0174 (3) | |
| H3A | 0.2982 | 0.5254 | 1.1744 | 0.021* | |
| C4 | 0.29766 (9) | 0.4723 (2) | 1.05606 (13) | 0.0206 (4) | |
| H4A | 0.3410 | 0.4226 | 1.0859 | 0.025* | |
| C5 | 0.26085 (9) | 0.4833 (2) | 0.95923 (13) | 0.0212 (4) | |
| H5A | 0.2802 | 0.4424 | 0.9257 | 0.025* | |
| C6 | 0.19723 (9) | 0.5525 (2) | 0.91211 (12) | 0.0174 (3) | |
| H6A | 0.1723 | 0.5610 | 0.8469 | 0.021* | |
| C7 | 0.17168 (8) | 0.6091 (2) | 0.96517 (11) | 0.0150 (3) | |
| C8 | 0.05184 (8) | 0.6967 (2) | 0.84619 (11) | 0.0163 (3) | |
| H8A | 0.0663 | 0.7624 | 0.8105 | 0.020* | |
| H8B | 0.0157 | 0.7582 | 0.8480 | 0.020* | |
| C9 | 0.02370 (8) | 0.5336 (2) | 0.79767 (11) | 0.0151 (3) | |
| C10 | 0.04406 (8) | 0.3851 (2) | 0.84445 (12) | 0.0178 (3) | |

| | | | | |
|---|---|---|---|---|
| H10A | 0.0740 | 0.3845 | 0.9093 | 0.021* |
| C11 | 0.02104 (9) | 0.2372 (2) | 0.79734 (12) | 0.0200 (4) |
| H11A | 0.0342 | 0.1364 | 0.8301 | 0.024* |
| C12 | 0.18631 (9) | 0.6741 (2) | 1.18835 (11) | 0.0186 (3) |
| H12A | 0.2176 | 0.7675 | 1.2179 | 0.022* |
| H12B | 0.2104 | 0.5727 | 1.2208 | 0.022* |
| C13 | 0.12542 (9) | 0.6968 (2) | 1.19816 (13) | 0.0212 (4) |
| H13A | 0.1402 | 0.7015 | 1.2636 | 0.032* |
| H13B | 0.0944 | 0.6044 | 1.1692 | 0.032* |
| H13C | 0.1024 | 0.7992 | 1.1681 | 0.032* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| P1 | 0.0129 (2) | 0.0162 (2) | 0.0174 (2) | 0.00054 (16) | 0.00725 (17) | 0.00099 (17) |
| F5 | 0.0197 (5) | 0.0208 (5) | 0.0221 (5) | 0.0054 (4) | 0.0084 (4) | 0.0053 (4) |
| F6 | 0.0233 (6) | 0.0279 (6) | 0.0390 (7) | 0.0116 (5) | 0.0115 (5) | 0.0080 (5) |
| F1 | 0.0212 (8) | 0.0261 (7) | 0.0505 (14) | −0.0047 (6) | 0.0224 (9) | −0.0001 (7) |
| F2 | 0.0303 (9) | 0.0381 (9) | 0.0169 (6) | 0.0070 (7) | 0.0083 (6) | −0.0039 (6) |
| F3 | 0.0263 (9) | 0.0207 (8) | 0.0519 (15) | −0.0042 (7) | 0.0244 (11) | 0.0045 (10) |
| F4 | 0.0382 (11) | 0.0331 (9) | 0.0228 (7) | 0.0058 (8) | 0.0157 (7) | −0.0062 (6) |
| N1 | 0.0127 (6) | 0.0161 (7) | 0.0134 (6) | 0.0006 (5) | 0.0056 (5) | −0.0010 (5) |
| N2 | 0.0112 (6) | 0.0185 (7) | 0.0137 (6) | 0.0007 (5) | 0.0044 (5) | −0.0010 (6) |
| C1 | 0.0122 (7) | 0.0179 (8) | 0.0151 (7) | 0.0008 (6) | 0.0057 (6) | −0.0011 (6) |
| C2 | 0.0126 (7) | 0.0133 (7) | 0.0157 (7) | −0.0015 (6) | 0.0067 (6) | −0.0014 (6) |
| C3 | 0.0132 (8) | 0.0175 (8) | 0.0175 (8) | 0.0002 (6) | 0.0051 (7) | 0.0007 (7) |
| C4 | 0.0131 (8) | 0.0216 (9) | 0.0238 (9) | 0.0034 (7) | 0.0074 (7) | 0.0021 (7) |
| C5 | 0.0198 (9) | 0.0219 (9) | 0.0268 (9) | 0.0000 (7) | 0.0155 (8) | −0.0023 (8) |
| C6 | 0.0168 (8) | 0.0189 (8) | 0.0161 (8) | −0.0025 (6) | 0.0082 (7) | −0.0023 (7) |
| C7 | 0.0112 (7) | 0.0142 (8) | 0.0165 (8) | −0.0017 (6) | 0.0050 (6) | −0.0009 (6) |
| C8 | 0.0117 (7) | 0.0202 (8) | 0.0114 (7) | −0.0004 (6) | 0.0022 (6) | 0.0006 (6) |
| C9 | 0.0102 (7) | 0.0201 (8) | 0.0143 (8) | −0.0008 (6) | 0.0059 (6) | −0.0009 (6) |
| C10 | 0.0117 (8) | 0.0235 (9) | 0.0147 (8) | −0.0010 (6) | 0.0045 (6) | 0.0018 (7) |
| C11 | 0.0146 (8) | 0.0191 (8) | 0.0227 (9) | 0.0014 (6) | 0.0072 (7) | 0.0042 (7) |
| C12 | 0.0193 (8) | 0.0216 (9) | 0.0121 (7) | 0.0021 (7) | 0.0062 (7) | −0.0011 (7) |
| C13 | 0.0260 (9) | 0.0195 (9) | 0.0227 (9) | 0.0017 (7) | 0.0158 (8) | 0.0017 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| P1—F2A | 1.481 (14) | C4—C5 | 1.410 (3) |
| P1—F3A | 1.552 (19) | C4—H4A | 0.9500 |
| P1—F4 | 1.5947 (14) | C5—C6 | 1.382 (2) |
| P1—F3 | 1.5957 (18) | C5—H5A | 0.9500 |
| P1—F1 | 1.5987 (13) | C6—C7 | 1.390 (2) |
| P1—F6 | 1.6011 (12) | C6—H6A | 0.9500 |
| P1—F2 | 1.6077 (15) | C8—C9 | 1.522 (2) |
| P1—F5 | 1.6082 (11) | C8—H8A | 0.9900 |
| P1—F1A | 1.656 (11) | C8—H8B | 0.9900 |
| P1—F4A | 1.674 (14) | C9—C10 | 1.390 (2) |
| N1—C1 | 1.330 (2) | C9—C9$^{i}$ | 1.409 (3) |

| | | | |
|---|---|---|---|
| N1—C2 | 1.397 (2) | C10—C11 | 1.391 (3) |
| N1—C12 | 1.478 (2) | C10—H10A | 0.9500 |
| N2—C1 | 1.337 (2) | C11—C11$^{i}$ | 1.383 (3) |
| N2—C7 | 1.395 (2) | C11—H11A | 0.9500 |
| N2—C8 | 1.467 (2) | C12—C13 | 1.518 (2) |
| C1—H1A | 0.9500 | C12—H12A | 0.9900 |
| C2—C7 | 1.392 (2) | C12—H12B | 0.9900 |
| C2—C3 | 1.395 (2) | C13—H13A | 0.9800 |
| C3—C4 | 1.383 (2) | C13—H13B | 0.9800 |
| C3—H3A | 0.9500 | C13—H13C | 0.9800 |

| | | | |
|---|---|---|---|
| F2A—P1—F3A | 95.5 (8) | N1—C1—H1A | 124.8 |
| F2A—P1—F4 | 157.6 (7) | N2—C1—H1A | 124.8 |
| F3A—P1—F4 | 106.7 (6) | C7—C2—C3 | 121.92 (15) |
| F2A—P1—F3 | 111.9 (7) | C7—C2—N1 | 106.67 (14) |
| F4—P1—F3 | 90.44 (11) | C3—C2—N1 | 131.37 (15) |
| F2A—P1—F1 | 67.6 (7) | C4—C3—C2 | 115.88 (16) |
| F3A—P1—F1 | 162.7 (6) | C4—C3—H3A | 122.1 |
| F4—P1—F1 | 90.05 (9) | C2—C3—H3A | 122.1 |
| F3—P1—F1 | 179.50 (11) | C3—C4—C5 | 122.29 (16) |
| F2A—P1—F6 | 88.8 (6) | C3—C4—H4A | 118.9 |
| F3A—P1—F6 | 86.5 (7) | C5—C4—H4A | 118.9 |
| F4—P1—F6 | 89.14 (8) | C6—C5—C4 | 121.35 (16) |
| F3—P1—F6 | 90.47 (9) | C6—C5—H5A | 119.3 |
| F1—P1—F6 | 89.39 (7) | C4—C5—H5A | 119.3 |
| F3A—P1—F2 | 73.4 (6) | C5—C6—C7 | 116.48 (16) |
| F4—P1—F2 | 179.76 (10) | C5—C6—H6A | 121.8 |
| F3—P1—F2 | 89.66 (11) | C7—C6—H6A | 121.8 |
| F1—P1—F2 | 89.86 (9) | C6—C7—C2 | 122.06 (15) |
| F6—P1—F2 | 91.07 (7) | C6—C7—N2 | 131.37 (16) |
| F2A—P1—F5 | 91.4 (6) | C2—C7—N2 | 106.53 (14) |
| F3A—P1—F5 | 93.4 (7) | N2—C8—C9 | 112.54 (14) |
| F4—P1—F5 | 90.69 (7) | N2—C8—H8A | 109.1 |
| F3—P1—F5 | 89.39 (9) | C9—C8—H8A | 109.1 |
| F1—P1—F5 | 90.75 (7) | N2—C8—H8B | 109.1 |
| F6—P1—F5 | 179.78 (9) | C9—C8—H8B | 109.1 |
| F2—P1—F5 | 89.10 (7) | H8A—C8—H8B | 107.8 |
| F2A—P1—F1A | 92.3 (7) | C10—C9—C9$^{i}$ | 119.25 (10) |
| F3A—P1—F1A | 171.2 (7) | C10—C9—C8 | 121.89 (14) |
| F4—P1—F1A | 65.9 (5) | C9$^{i}$—C9—C8 | 118.85 (9) |
| F3—P1—F1A | 154.6 (5) | C9—C10—C11 | 120.70 (15) |
| F6—P1—F1A | 97.8 (4) | C9—C10—H10A | 119.6 |
| F2—P1—F1A | 114.0 (5) | C11—C10—H10A | 119.7 |
| F5—P1—F1A | 82.2 (4) | C11$^{i}$—C11—C10 | 119.87 (10) |
| F2A—P1—F4A | 175.5 (8) | C11$^{i}$—C11—H11A | 120.1 |
| F3A—P1—F4A | 86.9 (7) | C10—C11—H11A | 120.1 |
| F3—P1—F4A | 70.3 (5) | N1—C12—C13 | 112.13 (14) |
| F1—P1—F4A | 110.2 (5) | N1—C12—H12A | 109.2 |
| F6—P1—F4A | 95.2 (5) | C13—C12—H12A | 109.2 |

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| F2—P1—F4A | 159.0 (6) | N1—C12—H12B | 109.2 |
| F5—P1—F4A | 84.6 (5) | C13—C12—H12B | 109.2 |
| F1A—P1—F4A | 85.1 (6) | H12A—C12—H12B | 107.9 |
| C1—N1—C2 | 108.21 (13) | C12—C13—H13A | 109.5 |
| C1—N1—C12 | 127.07 (14) | C12—C13—H13B | 109.5 |
| C2—N1—C12 | 124.68 (14) | H13A—C13—H13B | 109.5 |
| C1—N2—C7 | 108.18 (14) | C12—C13—H13C | 109.5 |
| C1—N2—C8 | 125.72 (14) | H13A—C13—H13C | 109.5 |
| C7—N2—C8 | 125.88 (14) | H13B—C13—H13C | 109.5 |
| N1—C1—N2 | 110.39 (14) | | |

| | | | |
|---|---|---|---|
| C2—N1—C1—N2 | −0.89 (19) | N1—C2—C7—C6 | −178.67 (15) |
| C12—N1—C1—N2 | −178.83 (15) | C3—C2—C7—N2 | 177.24 (15) |
| C7—N2—C1—N1 | 0.45 (19) | N1—C2—C7—N2 | −0.69 (18) |
| C8—N2—C1—N1 | 175.33 (15) | C1—N2—C7—C6 | 177.89 (18) |
| C1—N1—C2—C7 | 0.97 (18) | C8—N2—C7—C6 | 3.0 (3) |
| C12—N1—C2—C7 | 178.98 (15) | C1—N2—C7—C2 | 0.18 (18) |
| C1—N1—C2—C3 | −176.69 (18) | C8—N2—C7—C2 | −174.70 (15) |
| C12—N1—C2—C3 | 1.3 (3) | C1—N2—C8—C9 | −109.15 (18) |
| C7—C2—C3—C4 | −0.5 (2) | C7—N2—C8—C9 | 64.8 (2) |
| N1—C2—C3—C4 | 176.88 (17) | N2—C8—C9—C10 | 9.8 (2) |
| C2—C3—C4—C5 | 1.2 (3) | N2—C8—C9—C9$^{i}$ | −169.32 (17) |
| C3—C4—C5—C6 | −0.8 (3) | C9$^{i}$—C9—C10—C11 | 3.6 (3) |
| C4—C5—C6—C7 | −0.4 (3) | C8—C9—C10—C11 | −175.57 (16) |
| C5—C6—C7—C2 | 1.2 (3) | C9—C10—C11—C11$^{i}$ | 1.8 (3) |
| C5—C6—C7—N2 | −176.25 (17) | C1—N1—C12—C13 | 15.8 (2) |
| C3—C2—C7—C6 | −0.7 (3) | C2—N1—C12—C13 | −161.87 (15) |

Symmetry code: (i) −*x*, *y*, −*z*+3/2.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1*A*···F6$^{ii}$ | 0.95 | 2.42 | 3.142 (3) | 133 |
| C3—H3*A*···F5$^{iii}$ | 0.95 | 2.45 | 3.374 (2) | 166 |
| C5—H5*A*···F5$^{iv}$ | 0.95 | 2.52 | 3.420 (3) | 159 |
| C6—H6*A*···F4$^{v}$ | 0.95 | 2.53 | 3.392 (2) | 151 |
| C8—H8*B*···F1$^{ii}$ | 0.99 | 2.39 | 3.350 (3) | 164 |
| C13—H13*C*···F1$^{vi}$ | 0.98 | 2.55 | 3.523 (2) | 174 |
| C13—H13*C*···F5$^{vi}$ | 0.98 | 2.50 | 3.166 (2) | 125 |

Symmetry codes: (ii) *x*−1, *y*, *z*; (iii) *x*−1/2, −*y*+3/2, *z*+1/2; (iv) *x*−1/2, *y*−1/2, *z*; (v) −*x*+1, *y*, −*z*+3/2; (vi) −*x*+1, −*y*+2, −*z*+2.