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1-{2-[2-(1*H*-Benzimidazol-1-yl)ethoxy]-ethyl}-1*H*-benzimidazol-3-ium hexafluorophosphate

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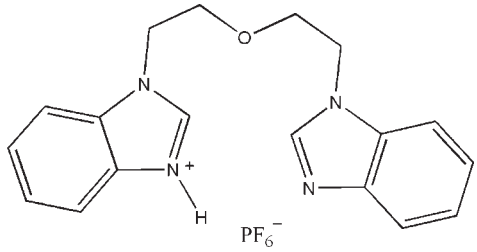
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.002 Å; disorder in solvent or counterion; R factor = 0.040; wR factor = 0.080; data-to-parameter ratio = 13.1.

In the title salt, $C_{18}H_{19}N_4O^+\cdot PF_6^-$, the dihedral angle between the benzimidazolium and benzimidazole ring systems is 16.24 (2)°. In the cation, a π–π interaction is observed between the imidazolium ring and the benzene ring of the benzimidazole ring system [centroid–centroid distance = 3.5713 (11) Å]. The PF_6^- ion is disordered over two sites, with occupancies of 0.895 (2) and 0.105 (2). In the crystal structure, pairs of N—H···N hydrogen bonds link the cations, forming centrosymmetric dimers. The dimers are linked *via* π–π interactions [centroid–centroid distance = 3.5606 (11) Å]. In addition, C—H···F hydrogen bonds are observed.

Related literature

For the synthesis, see: Zeng *et al.* (2008). For general background to benzimidazole derivatives, see: Pal *et al.* (2007); Murru *et al.* (2009).



Experimental

Crystal data

$C_{18}H_{19}N_4O^+\cdot PF_6^-$
M_r = 452.34
Monoclinic, $P2_1/c$
a = 10.5347 (18) Å
b = 13.771 (2) Å
c = 13.353 (2) Å
β = 92.507 (2)°
V = 1935.3 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 93 K
0.37 × 0.33 × 0.27 mm

Data collection

Rigaku SPIDER diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.923, T_{max} = 0.943
11885 measured reflections
3959 independent reflections
3445 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
Standard reflections: 0

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.080
S = 1.00
3959 reflections
303 parameters
21 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···N4^{i}	1.05 (2)	1.68 (2)	2.724 (2)	176 (2)
C4—H4···F3^{ii}	0.95	2.41	3.130 (2)	133
C7—H7···F4^{iii}	0.95	2.23	3.100 (2)	152
C9—H9*B*···F2^{iii}	0.99	2.40	3.340 (2)	159
C11—H11*A*···F2^{iv}	0.99	2.51	3.066 (2)	116
C16—H16···F4^{v}	0.95	2.39	3.300 (2)	161
C18—H18···F6	0.95	2.38	3.298 (2)	163

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

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5075).

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supplementary materials

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1-{2-[2-(1*H*-Benzimidazol-1-yl)ethoxy]ethyl}-1*H*-benzimidazol-3-ium hexafluorophosphate

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Comment

Benzimidazole derivatives are an important class of heterocycles that are present in a number of biologically active compounds. These derivatives are also used as cyclic N-heterocyclic carbene (NHC) precursors (Murru *et al.*, 2009). A benzimidazole N-donor dinuclear palladacycle complex is used as an efficient Suzuki coupling catalyst (Pal *et al.*, 2007).

Bond lengths and angles in the ionic pairs (Fig. 1) are within normal ranges. The benzimidazolium and benzimidazole ring systems make a dihedral angle of 16.24 (2)°. In the cation, a π–π interaction is observed between N1/C1/C6/N2C7 and C12-C17 rings, with the ring centroids being separated by 3.5713 (11) Å.

In the crystal structure, pairs of N—H···N hydrogen bonds link cations to form centrosymmetric dimers. The dimers are linked via π–π interactions between the N1/C1/C6/N2C7 ring at (x, y, z) and the C12-C17 ring at (1-x, y-1/2, 1/2-z), with their centroids separated by 3.5606 (11) Å. In addition, C—H···F hydrogen bonds are observed (Table 1).

Experimental

The title compound was prepared according to the reported procedure of Zeng *et al.*. (2008). Colourless single crystals suitable for X-ray diffraction were obtained by recrystallization from acetonitrile and ethyl ether.

Refinement

The PF_6^- ion is disordered over two sites with occupancies of 0.895 (2) and 0.105 (2). The U^{ij} values of atom pairs F1/F1', F2/F2', F3/F3, F4/F4', F5/F5' and F6/F6' were constrained to be equal. The corresponding distances in the two disorder components were restrained to be the same. Atom H1N was located in a difference map and refined freely. All other H atoms were placed in calculated positions [C–H = 0.95–0.99 Å] and refined in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

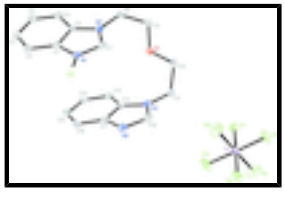


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. C-bound H atoms have been omitted. For clarity, only the major disorder component is shown.

1-{2-[2-(1*H*-Benzimidazol-1-yl)ethoxy]ethyl}-1*H*- benzimidazol-3-ium hexafluorophosphate

Crystal data

$C_{18}H_{19}N_4O^+ \cdot PF_6^-$	$F(000) = 928$
$M_r = 452.34$	$D_x = 1.553$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 5714 reflections
$a = 10.5347$ (18) Å	$\theta = 3.1$–$27.5°$
$b = 13.771$ (2) Å	$\mu = 0.22$ mm^{-1}
$c = 13.353$ (2) Å	$T = 93$ K
$\beta = 92.507$ (2)°	Block, colourless
$V = 1935.3$ (6) Å^3	0.37 × 0.33 × 0.27 mm
$Z = 4$	

Data collection

Rigaku SPIDER diffractometer	3959 independent reflections
Radiation source: Rotating Anode	3445 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.026$
ω scans	$\theta_{max} = 26.4°$, $\theta_{min} = 3.1°$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -13 \rightarrow 10$
$T_{min} = 0.923$, $T_{max} = 0.943$	$k = -13 \rightarrow 17$
11885 measured reflections	$l = -15 \rightarrow 16$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.040$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.080$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.0259P)^2 + 0.968P]$ where $P = (F_o^2 + 2F_c^2)/3$
3959 reflections	$(\Delta/\sigma)_{max} = 0.001$
303 parameters	$\Delta\rho_{max} = 0.34$ e Å^{-3}
21 restraints	$\Delta\rho_{min} = -0.28$ 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 $F^2 > \sigma(F^2)$ 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_{iso}*/U_{eq}	Occ. (<1)
O1	0.20360 (11)	0.51931 (8)	0.18156 (8)	0.0247 (3)	
N1	0.53426 (13)	0.40531 (10)	0.31178 (10)	0.0243 (3)	
N2	0.41920 (13)	0.39824 (9)	0.17089 (10)	0.0218 (3)	
N3	0.26475 (13)	0.62988 (10)	0.35541 (10)	0.0253 (3)	
N4	0.39492 (14)	0.60700 (10)	0.48994 (10)	0.0294 (3)	
C1	0.61864 (16)	0.39760 (11)	0.23507 (12)	0.0229 (3)	
C2	0.75022 (16)	0.39314 (12)	0.23627 (13)	0.0285 (4)	
H2	0.8005	0.3964	0.2970	0.034*	
C3	0.80419 (17)	0.38372 (13)	0.14435 (14)	0.0319 (4)	
H3	0.8941	0.3801	0.1420	0.038*	
C4	0.73059 (17)	0.37927 (13)	0.05438 (13)	0.0311 (4)	
H4	0.7718	0.3730	−0.0072	0.037*	
C5	0.60018 (16)	0.38377 (12)	0.05330 (12)	0.0262 (4)	
H5	0.5499	0.3808	−0.0075	0.031*	
C6	0.54567 (15)	0.39293 (11)	0.14572 (12)	0.0218 (3)	
C7	0.41753 (16)	0.40521 (11)	0.27069 (12)	0.0245 (4)	
H7	0.3424	0.4095	0.3073	0.029*	
C8	0.31129 (15)	0.39532 (12)	0.09736 (12)	0.0242 (4)	
H8A	0.3030	0.3288	0.0698	0.029*	
H8B	0.3286	0.4397	0.0412	0.029*	
C9	0.18818 (16)	0.42403 (12)	0.14171 (13)	0.0262 (4)	
H9A	0.1185	0.4231	0.0895	0.031*	
H9B	0.1668	0.3780	0.1954	0.031*	
C10	0.10406 (16)	0.54786 (12)	0.24439 (12)	0.0272 (4)	
H10A	0.0890	0.4968	0.2947	0.033*	
H10B	0.0243	0.5584	0.2039	0.033*	
C11	0.14574 (16)	0.64079 (13)	0.29557 (12)	0.0277 (4)	
H11A	0.1568	0.6916	0.2442	0.033*	
H11B	0.0783	0.6627	0.3397	0.033*	
C12	0.38716 (16)	0.64002 (11)	0.32253 (12)	0.0231 (3)	
C13	0.43309 (16)	0.65920 (12)	0.22830 (12)	0.0262 (4)	
H13	0.3775	0.6687	0.1712	0.031*	
C14	0.56322 (17)	0.66369 (12)	0.22204 (13)	0.0295 (4)	
H14	0.5982	0.6764	0.1590	0.035*	
C15	0.64530 (18)	0.64993 (12)	0.30653 (14)	0.0314 (4)	
H15	0.7345	0.6539	0.2994	0.038*	
C16	0.59940 (17)	0.63079 (12)	0.39979 (13)	0.0294 (4)	
H16	0.6553	0.6214	0.4567	0.035*	

C17	0.46803 (17)	0.62576 (11)	0.40726 (12)	0.0249 (4)	
C18	0.27606 (18)	0.61067 (13)	0.45479 (12)	0.0299 (4)	
H18	0.2053	0.6008	0.4953	0.036*	
P1	−0.07196 (5)	0.71567 (4)	0.57610 (4)	0.02117 (17)	0.8952 (16)
F1	−0.10379 (15)	0.71525 (12)	0.45828 (8)	0.0350 (3)	0.8952 (16)
F2	−0.03912 (12)	0.71374 (11)	0.69440 (8)	0.0393 (4)	0.8952 (16)
F3	0.05729 (13)	0.77151 (12)	0.55925 (10)	0.0540 (4)	0.8952 (16)
F4	−0.19885 (12)	0.65494 (12)	0.59425 (9)	0.0479 (4)	0.8952 (16)
F5	−0.14535 (18)	0.81437 (11)	0.58739 (10)	0.0589 (5)	0.8952 (16)
F6	0.00255 (14)	0.61439 (10)	0.56578 (10)	0.0509 (4)	0.8952 (16)
P1'	−0.0834 (6)	0.7250 (5)	0.5725 (5)	0.141 (8)	0.1048 (16)
F1'	−0.0918 (11)	0.7157 (9)	0.4533 (4)	0.0350 (3)	0.1048 (16)
F2'	−0.0730 (10)	0.7334 (8)	0.6921 (5)	0.0393 (4)	0.1048 (16)
F3'	−0.0180 (10)	0.8283 (6)	0.5636 (8)	0.0540 (4)	0.1048 (16)
F4'	−0.1434 (9)	0.6186 (6)	0.5824 (8)	0.0479 (4)	0.1048 (16)
F5'	−0.2196 (8)	0.7721 (8)	0.5714 (8)	0.0589 (5)	0.1048 (16)
F6'	0.0549 (7)	0.6755 (8)	0.5745 (8)	0.0509 (4)	0.1048 (16)
H1N	0.560 (2)	0.4037 (15)	0.3887 (16)	0.052 (6)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0252 (6)	0.0252 (6)	0.0238 (6)	−0.0009 (5)	0.0013 (5)	−0.0021 (5)
N1	0.0294 (8)	0.0246 (7)	0.0183 (7)	0.0024 (6)	−0.0043 (6)	−0.0007 (6)
N2	0.0255 (7)	0.0219 (7)	0.0177 (6)	0.0001 (6)	−0.0024 (5)	−0.0005 (5)
N3	0.0272 (8)	0.0310 (8)	0.0175 (7)	0.0061 (6)	−0.0033 (6)	−0.0007 (6)
N4	0.0360 (9)	0.0325 (8)	0.0192 (7)	0.0027 (6)	−0.0050 (6)	0.0010 (6)
C1	0.0294 (9)	0.0190 (8)	0.0200 (8)	0.0016 (6)	−0.0023 (7)	−0.0006 (6)
C2	0.0285 (9)	0.0297 (9)	0.0266 (9)	0.0011 (7)	−0.0083 (7)	0.0012 (7)
C3	0.0248 (9)	0.0350 (10)	0.0357 (10)	0.0030 (7)	0.0004 (8)	0.0041 (8)
C4	0.0323 (10)	0.0361 (10)	0.0252 (9)	0.0054 (8)	0.0048 (8)	0.0035 (8)
C5	0.0319 (10)	0.0281 (9)	0.0184 (8)	0.0021 (7)	−0.0026 (7)	0.0003 (7)
C6	0.0246 (9)	0.0180 (8)	0.0225 (8)	0.0011 (6)	−0.0026 (7)	−0.0001 (6)
C7	0.0301 (9)	0.0235 (8)	0.0198 (8)	0.0017 (7)	0.0007 (7)	−0.0002 (7)
C8	0.0261 (9)	0.0254 (9)	0.0204 (8)	−0.0013 (7)	−0.0059 (7)	−0.0011 (7)
C9	0.0259 (9)	0.0268 (9)	0.0255 (9)	−0.0024 (7)	−0.0030 (7)	−0.0015 (7)
C10	0.0230 (9)	0.0346 (10)	0.0240 (9)	0.0024 (7)	0.0012 (7)	0.0020 (7)
C11	0.0249 (9)	0.0357 (10)	0.0222 (8)	0.0076 (7)	−0.0027 (7)	−0.0003 (7)
C12	0.0281 (9)	0.0199 (8)	0.0207 (8)	0.0022 (7)	−0.0044 (7)	−0.0031 (6)
C13	0.0329 (10)	0.0262 (9)	0.0189 (8)	−0.0019 (7)	−0.0055 (7)	−0.0033 (7)
C14	0.0347 (10)	0.0285 (9)	0.0254 (9)	−0.0061 (7)	0.0015 (8)	−0.0051 (7)
C15	0.0288 (10)	0.0287 (9)	0.0362 (10)	−0.0045 (7)	−0.0039 (8)	−0.0048 (8)
C16	0.0332 (10)	0.0246 (9)	0.0294 (9)	−0.0008 (7)	−0.0120 (8)	−0.0027 (7)
C17	0.0325 (9)	0.0202 (8)	0.0212 (8)	0.0013 (7)	−0.0056 (7)	−0.0019 (6)
C18	0.0360 (10)	0.0346 (10)	0.0189 (8)	0.0048 (8)	−0.0004 (7)	0.0013 (7)
P1	0.0156 (3)	0.0302 (3)	0.0175 (4)	−0.0041 (2)	−0.0011 (2)	0.0053 (3)
F1	0.0370 (7)	0.0499 (7)	0.0182 (5)	0.0021 (5)	0.0012 (4)	0.0020 (5)
F2	0.0360 (9)	0.0587 (9)	0.0220 (5)	−0.0174 (6)	−0.0105 (5)	0.0105 (5)

F3	0.0427 (9)	0.0789 (11)	0.0405 (8)	−0.0350 (8)	0.0021 (6)	0.0096 (7)
F4	0.0266 (8)	0.0901 (11)	0.0269 (6)	−0.0273 (7)	−0.0006 (6)	0.0019 (7)
F5	0.0895 (13)	0.0551 (10)	0.0322 (8)	0.0370 (9)	0.0014 (8)	−0.0026 (7)
F6	0.0558 (9)	0.0451 (9)	0.0519 (8)	0.0174 (7)	0.0044 (7)	0.0118 (7)
P1'	0.167 (16)	0.22 (2)	0.030 (7)	−0.026 (15)	−0.032 (8)	0.006 (9)
F1'	0.0370 (7)	0.0499 (7)	0.0182 (5)	0.0021 (5)	0.0012 (4)	0.0020 (5)
F2'	0.0360 (9)	0.0587 (9)	0.0220 (5)	−0.0174 (6)	−0.0105 (5)	0.0105 (5)
F3'	0.0427 (9)	0.0789 (11)	0.0405 (8)	−0.0350 (8)	0.0021 (6)	0.0096 (7)
F4'	0.0266 (8)	0.0901 (11)	0.0269 (6)	−0.0273 (7)	−0.0006 (6)	0.0019 (7)
F5'	0.0895 (13)	0.0551 (10)	0.0322 (8)	0.0370 (9)	0.0014 (8)	−0.0026 (7)
F6'	0.0558 (9)	0.0451 (9)	0.0519 (8)	0.0174 (7)	0.0044 (7)	0.0118 (7)

Geometric parameters (Å, °)

O1—C9	1.4224 (19)	C10—C11	1.507 (2)
O1—C10	1.4266 (19)	C10—H10A	0.99
N1—C7	1.325 (2)	C10—H10B	0.99
N1—C1	1.389 (2)	C11—H11A	0.99
N1—H1N	1.05 (2)	C11—H11B	0.99
N2—C7	1.337 (2)	C12—C13	1.393 (2)
N2—C6	1.390 (2)	C12—C17	1.400 (2)
N2—C8	1.470 (2)	C13—C14	1.378 (2)
N3—C18	1.353 (2)	C13—H13	0.95
N3—C12	1.387 (2)	C14—C15	1.404 (2)
N3—C11	1.465 (2)	C14—H14	0.95
N4—C18	1.319 (2)	C15—C16	1.381 (3)
N4—C17	1.398 (2)	C15—H15	0.95
C1—C2	1.387 (2)	C16—C17	1.394 (2)
C1—C6	1.392 (2)	C16—H16	0.95
C2—C3	1.381 (2)	C18—H18	0.95
C2—H2	0.95	P1—F5	1.5742 (14)
C3—C4	1.402 (3)	P1—F3	1.5883 (13)
C3—H3	0.95	P1—F1	1.5942 (12)
C4—C5	1.375 (2)	P1—F2	1.6025 (12)
C4—H4	0.95	P1—F4	1.6041 (12)
C5—C6	1.389 (2)	P1—F6	1.6092 (14)
C5—H5	0.95	P1'—F5'	1.574 (3)
C7—H7	0.95	P1'—F3'	1.588 (3)
C8—C9	1.502 (2)	P1'—F1'	1.595 (3)
C8—H8A	0.99	P1'—F2'	1.601 (3)
C8—H8B	0.99	P1'—F4'	1.603 (3)
C9—H9A	0.99	P1'—F6'	1.608 (3)
C9—H9B	0.99		
C9—O1—C10	113.54 (12)	C10—C11—H11B	109.1
C7—N1—C1	107.87 (14)	H11A—C11—H11B	107.8
C7—N1—H1N	126.9 (11)	N3—C12—C13	132.02 (15)
C1—N1—H1N	125.0 (11)	N3—C12—C17	105.74 (14)
C7—N2—C6	107.41 (13)	C13—C12—C17	122.24 (16)
C7—N2—C8	128.63 (14)	C14—C13—C12	116.68 (16)

C6—N2—C8	123.95 (13)	C14—C13—H13	121.7
C18—N3—C12	106.67 (14)	C12—C13—H13	121.7
C18—N3—C11	126.26 (15)	C13—C14—C15	121.63 (16)
C12—N3—C11	127.04 (13)	C13—C14—H14	119.2
C18—N4—C17	105.03 (14)	C15—C14—H14	119.2
C2—C1—N1	131.78 (15)	C16—C15—C14	121.52 (17)
C2—C1—C6	121.47 (15)	C16—C15—H15	119.2
N1—C1—C6	106.75 (14)	C14—C15—H15	119.2
C3—C2—C1	116.36 (16)	C15—C16—C17	117.52 (16)
C3—C2—H2	121.8	C15—C16—H16	121.2
C1—C2—H2	121.8	C17—C16—H16	121.2
C2—C3—C4	122.12 (17)	C16—C17—N4	130.48 (16)
C2—C3—H3	118.9	C16—C17—C12	120.41 (16)
C4—C3—H3	118.9	N4—C17—C12	109.11 (15)
C5—C4—C3	121.46 (16)	N4—C18—N3	113.45 (16)
C5—C4—H4	119.3	N4—C18—H18	123.3
C3—C4—H4	119.3	N3—C18—H18	123.3
C4—C5—C6	116.52 (16)	F5—P1—F3	91.33 (10)
C4—C5—H5	121.7	F5—P1—F1	90.84 (8)
C6—C5—H5	121.7	F3—P1—F1	90.37 (7)
C5—C6—N2	131.09 (15)	F5—P1—F2	90.33 (7)
C5—C6—C1	122.08 (15)	F3—P1—F2	89.90 (7)
N2—C6—C1	106.83 (14)	F1—P1—F2	178.79 (8)
N1—C7—N2	111.14 (15)	F5—P1—F4	91.13 (10)
N1—C7—H7	124.4	F3—P1—F4	177.42 (10)
N2—C7—H7	124.4	F1—P1—F4	90.37 (7)
N2—C8—C9	112.67 (13)	F2—P1—F4	89.30 (6)
N2—C8—H8A	109.1	F5—P1—F6	179.35 (8)
C9—C8—H8A	109.1	F3—P1—F6	89.03 (8)
N2—C8—H8B	109.1	F1—P1—F6	89.69 (8)
C9—C8—H8B	109.1	F2—P1—F6	89.14 (8)
H8A—C8—H8B	107.8	F4—P1—F6	88.51 (9)
O1—C9—C8	107.68 (13)	F5'—P1'—F3'	91.6 (3)
O1—C9—H9A	110.2	F5'—P1'—F1'	90.8 (3)
C8—C9—H9A	110.2	F3'—P1'—F1'	90.2 (3)
O1—C9—H9B	110.2	F5'—P1'—F2'	90.1 (3)
C8—C9—H9B	110.2	F3'—P1'—F2'	89.9 (3)
H9A—C9—H9B	108.5	F1'—P1'—F2'	179.1 (4)
O1—C10—C11	107.08 (13)	F5'—P1'—F4'	90.8 (3)
O1—C10—H10A	110.3	F3'—P1'—F4'	177.5 (4)
C11—C10—H10A	110.3	F1'—P1'—F4'	90.2 (3)
O1—C10—H10B	110.3	F2'—P1'—F4'	89.6 (3)
C11—C10—H10B	110.3	F5'—P1'—F6'	179.1 (4)
H10A—C10—H10B	108.6	F3'—P1'—F6'	89.2 (3)
N3—C11—C10	112.69 (14)	F1'—P1'—F6'	89.7 (3)
N3—C11—H11A	109.1	F2'—P1'—F6'	89.5 (3)
C10—C11—H11A	109.1	F4'—P1'—F6'	88.4 (3)
N3—C11—H11B	109.1		
C7—N1—C1—C2	−179.03 (17)	C9—O1—C10—C11	169.54 (13)

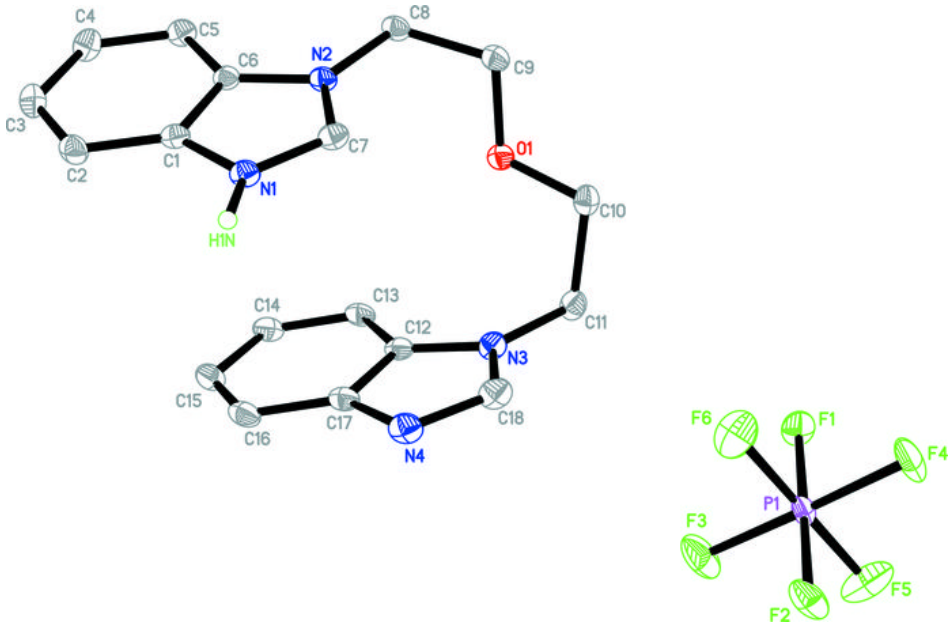
C7—N1—C1—C6	0.03 (17)	C18—N3—C11—C10	−94.78 (19)
N1—C1—C2—C3	178.85 (16)	C12—N3—C11—C10	87.35 (19)
C6—C1—C2—C3	−0.1 (2)	O1—C10—C11—N3	−58.98 (17)
C1—C2—C3—C4	0.3 (3)	C18—N3—C12—C13	179.45 (17)
C2—C3—C4—C5	−0.2 (3)	C11—N3—C12—C13	−2.3 (3)
C3—C4—C5—C6	0.0 (2)	C18—N3—C12—C17	0.01 (17)
C4—C5—C6—N2	−179.17 (16)	C11—N3—C12—C17	178.22 (15)
C4—C5—C6—C1	0.2 (2)	N3—C12—C13—C14	−179.43 (16)
C7—N2—C6—C5	179.09 (16)	C17—C12—C13—C14	−0.1 (2)
C8—N2—C6—C5	−0.4 (3)	C12—C13—C14—C15	−0.2 (2)
C7—N2—C6—C1	−0.31 (17)	C13—C14—C15—C16	0.3 (3)
C8—N2—C6—C1	−179.76 (13)	C14—C15—C16—C17	−0.1 (2)
C2—C1—C6—C5	−0.1 (2)	C15—C16—C17—N4	179.34 (16)
N1—C1—C6—C5	−179.29 (14)	C15—C16—C17—C12	−0.2 (2)
C2—C1—C6—N2	179.35 (14)	C18—N4—C17—C16	−179.82 (17)
N1—C1—C6—N2	0.17 (17)	C18—N4—C17—C12	−0.29 (18)
C1—N1—C7—N2	−0.23 (18)	N3—C12—C17—C16	179.76 (14)
C6—N2—C7—N1	0.34 (18)	C13—C12—C17—C16	0.3 (2)
C8—N2—C7—N1	179.76 (14)	N3—C12—C17—N4	0.17 (17)
C7—N2—C8—C9	13.2 (2)	C13—C12—C17—N4	−179.34 (14)
C6—N2—C8—C9	−167.43 (14)	C17—N4—C18—N3	0.31 (19)
C10—O1—C9—C8	−167.47 (13)	C12—N3—C18—N4	−0.21 (19)
N2—C8—C9—O1	58.10 (17)	C11—N3—C18—N4	−178.43 (15)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···N4^{i}	1.05 (2)	1.68 (2)	2.724 (2)	176 (2)
C4—H4···F3^{ii}	0.95	2.41	3.130 (2)	133
C7—H7···F4^{iii}	0.95	2.23	3.100 (2)	152
C9—H9B···F2^{iii}	0.99	2.40	3.340 (2)	159
C11—H11A···F2^{iv}	0.99	2.51	3.066 (2)	116
C16—H16···F4^{v}	0.95	2.39	3.300 (2)	161
C18—H18···F6	0.95	2.38	3.298 (2)	163

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

Fig. 1


C4
C5
C8
N2
C6
C9
C3
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O1
C1
C2
N1
C10
H1N
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C13
C11
C12
N3
C15
C17
C18
C16
N4
F6
F1
F4
P1
F3
F5
F2