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3-(8-Methoxyquinolin-2-ylmethyl)-1-methyl-3*H*-1-imidazolium hexafluorophosphate

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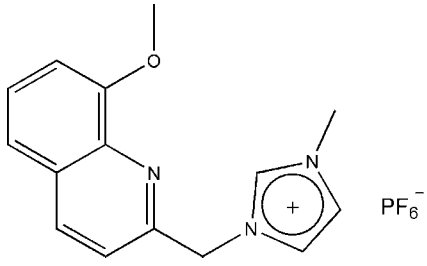
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.058; wR factor = 0.170; data-to-parameter ratio = 10.5.

In the cation of the title compound, $C_{15}H_{17}N_3O^+\cdot PF_6^-$, the dihedral angle between the mean planes of the quinoline and imidazole groups is 78.02 (7)°. In the crystal structure, π–π stacking interactions, with a ring centroid separation of 3.752 (2) Å, link the molecules into centrosymmetric dimers. In addition, weak intermolecular C—H···F and C—H···O interactions help to stabilize the crystal structure. The F atoms of the anion are disordered over two sites in a ratio of approximately 0.86:0.14.

Related literature

For related literature, see: Bortolini *et al.* (2003); Dibrov & Kochi (2006); Pretti *et al.* (2006).



Experimental

Crystal data

$C_{15}H_{17}N_3O^+\cdot F_6P^-$
M_r = 400.29
Monoclinic, $C2/c$
a = 12.2183 (11) Å
b = 21.3444 (19) Å
c = 14.4056 (13) Å
β = 112.059 (1)°
V = 3481.9 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 291 (2) K
0.24 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.947, T_{max} = 0.964
12564 measured reflections
3087 independent reflections
2808 reflections with $I > 2\sigma(I)$
R_{int} = 0.108

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.170
S = 1.05
3087 reflections
293 parameters
108 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···F1^{i}	0.93	2.46	3.204 (5)	137
C9—H9A···F2^{ii}	0.97	2.49	3.244 (4)	135
C3—H3···O1^{iii}	0.93	2.27	3.122 (3)	152

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *SHELXTL* (Bruker, 1998).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2402).

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supplementary materials

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3-(8-Methoxyquinolin-2-ylmethyl)-1-methyl-3*H*-1-imidazolium hexafluorophosphate

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Comment

Room-temperature ionic liquids are attracting significant interest owing to their chemical characteristics and potentially useful solvent properties (Dibrov & Kochi, 2006) and imidazolium salts, which are regarded as a type of ionic liquids, have an extensive application in organic synthesis (Pretti *et al.*, 2006).

The molecular structure of (I) is shown in Fig. 1. The dihedral angle between the quinoline plane and imidazole plane is 78.02 (7) °. In the crystal structure, π-π stacking internactions link molecules into centrosymmetric dimers. In addtion, weak intermolecular C—H···F and C—H···O interactions help stabilize the crystal structure.

Experimental

The title compound was synthesized according to the literature procedure (Bortolini *et al.*, 2003).

Refinement

All H atoms were included in calculated positions and refined as riding (C—H = 0.93–0.97 Å; N—H = 0.88 Å), with U_{iso}(H) = 1.5U_{eq}(C) for methyl and 1.2U_{eq}(C,*N*) for all other H atoms. The largest peak in the final difference Fourier of 1.33 e Å^{-3} is 0.83 Å from atom H7. The F atoms of the anion are disordered over two sites with refined occupancies 0.859 (6) and 0.141 (6) for the major and minor components.

Figures

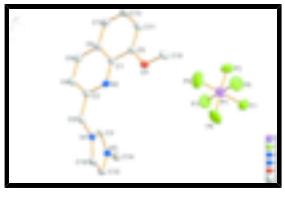

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids. Hydrogen atoms and the minor component of disorder have been omitted.

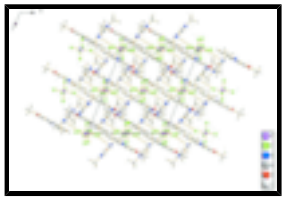

Fig. 2. : The packing of the title compound, viewed down the *b* axis.

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Crystal data

$C_{15}H_{17}N_3O^+·F_6P^-$	$Z = 8$
$M_r = 400.29$	$F_{000} = 1640$
Monoclinic, *C*2/*c*	$D_x = 1.527$ Mg m^{-3}
Hall symbol: -C 2yc	Mo *K*α radiation λ = 0.71073 Å
a = 12.2183 (11) Å	μ = 0.23 mm^{-1}
b = 21.3444 (19) Å	*T* = 291 (2) K
c = 14.4056 (13) Å	Block, colourless
β = 112.059 (1)º	0.24 × 0.18 × 0.16 mm
V = 3481.9 (5) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3087 independent reflections
Radiation source: fine-focus sealed tube	2808 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.108$
T = 291(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −14→13
$T_{min} = 0.947$, $T_{max} = 0.964$	*k* = −25→25
12564 measured reflections	*l* = −16→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.059$	H-atom parameters constrained
$wR(F^2) = 0.170$	$w = 1/[\sigma^2(F_o^2) + (0.0848P)^2 + 6.8821P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} = 0.001$
3087 reflections	$\Delta\rho_{max} = 1.13$ e Å^{-3}
293 parameters	$\Delta\rho_{min} = -0.67$ e Å^{-3}
108 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0026 (5)

Special details

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 $F^2 > 2\text{sigma}(F^2)$ 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)
P1	0.01910 (7)	0.33923 (4)	0.99358 (6)	0.0431 (3)	
F1	0.0575 (5)	0.3561 (2)	1.1098 (3)	0.092 (2)	0.859 (6)
F2	0.0141 (3)	0.26827 (11)	1.0220 (2)	0.0687 (9)	0.859 (6)
F3	−0.1135 (2)	0.3483 (2)	0.9796 (3)	0.0951 (13)	0.859 (6)
F4	0.0294 (4)	0.41165 (15)	0.9733 (3)	0.1144 (16)	0.859 (6)
F5	0.1552 (2)	0.33103 (19)	1.0130 (3)	0.0916 (12)	0.859 (6)
F6	−0.0185 (5)	0.3223 (3)	0.8809 (3)	0.118 (3)	0.859 (6)
F1'	0.0459 (14)	0.3516 (7)	1.1049 (6)	0.038 (6)	0.141 (6)
F2'	−0.0984 (11)	0.3001 (8)	0.9825 (10)	0.080 (6)	0.141 (6)
F3'	−0.0593 (16)	0.3991 (6)	0.9584 (11)	0.089 (7)	0.141 (6)
F4'	0.1291 (12)	0.3739 (9)	0.9927 (12)	0.113 (9)	0.141 (6)
F5'	0.0894 (16)	0.2751 (6)	1.0179 (12)	0.117 (9)	0.141 (6)
F6'	−0.0142 (12)	0.3222 (7)	0.8752 (7)	0.046 (6)	0.141 (6)
N1	0.35973 (18)	0.67281 (10)	0.14547 (16)	0.0286 (5)	
N2	0.51217 (19)	0.55385 (10)	0.12278 (15)	0.0297 (5)	
H2	0.5699	0.5799	0.1455	0.036*	
N3	0.29978 (19)	0.68579 (10)	0.26701 (16)	0.0324 (5)	
O1	0.73297 (16)	0.51432 (9)	0.21731 (16)	0.0406 (5)	
C1	0.5310 (2)	0.49095 (12)	0.13432 (18)	0.0302 (6)	
C2	0.4026 (2)	0.57384 (13)	0.07571 (19)	0.0326 (6)	
C3	0.3228 (2)	0.64369 (12)	0.20928 (19)	0.0305 (6)	
H3	0.3143	0.6006	0.2130	0.037*	
C4	0.3047 (2)	0.53339 (14)	0.0384 (2)	0.0403 (7)	
H4	0.2290	0.5494	0.0063	0.048*	
C5	0.6489 (2)	0.46864 (12)	0.1842 (2)	0.0336 (6)	
C6	0.3226 (3)	0.47019 (14)	0.0499 (2)	0.0407 (7)	
H6	0.2588	0.4429	0.0260	0.049*	
C7	0.4631 (3)	0.38144 (13)	0.1118 (2)	0.0410 (7)	
H7	0.4025	0.3522	0.0882	0.049*	
C8	0.4378 (2)	0.44646 (13)	0.09821 (19)	0.0338 (6)	
C9	0.3866 (3)	0.64389 (13)	0.0633 (2)	0.0360 (6)	
H9A	0.4582	0.6624	0.0612	0.043*	
H9B	0.3229	0.6528	0.0000	0.043*	

C10	0.3589 (3)	0.73643 (13)	0.1622 (2)	0.0385 (6)
H10	0.3799	0.7680	0.1275	0.046*
C11	0.6706 (3)	0.40540 (13)	0.1961 (2)	0.0407 (7)
H11	0.7475	0.3910	0.2284	0.049*
C12	0.3219 (3)	0.74401 (13)	0.2382 (2)	0.0401 (7)
H12	0.3130	0.7820	0.2663	0.048*
C13	0.5766 (3)	0.36226 (13)	0.1594 (2)	0.0436 (7)
H13	0.5927	0.3196	0.1680	0.052*
C14	0.2529 (3)	0.67183 (15)	0.3445 (2)	0.0460 (7)
H14A	0.1684	0.6752	0.3166	0.069*
H14B	0.2846	0.7011	0.3987	0.069*
H14C	0.2750	0.6300	0.3690	0.069*
C15	0.8535 (3)	0.49475 (17)	0.2664 (3)	0.0613 (10)
H15A	0.8622	0.4725	0.3266	0.092*
H15B	0.9040	0.5309	0.2827	0.092*
H15C	0.8749	0.4678	0.2226	0.092*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0324 (5)	0.0473 (5)	0.0488 (5)	−0.0030 (3)	0.0140 (3)	0.0112 (3)
F1	0.112 (4)	0.076 (3)	0.066 (3)	0.004 (3)	0.009 (2)	−0.017 (2)
F2	0.092 (2)	0.0408 (13)	0.0805 (18)	−0.0165 (13)	0.0406 (16)	−0.0023 (12)
F3	0.0347 (14)	0.126 (3)	0.115 (3)	0.0141 (16)	0.0167 (14)	−0.015 (2)
F4	0.113 (3)	0.068 (2)	0.128 (3)	−0.0150 (19)	0.006 (2)	0.0528 (19)
F5	0.0423 (15)	0.118 (3)	0.122 (3)	−0.0103 (16)	0.0385 (16)	0.007 (2)
F6	0.125 (5)	0.168 (5)	0.057 (3)	−0.007 (4)	0.029 (3)	0.003 (3)
F1'	0.047 (8)	0.035 (9)	0.034 (9)	0.004 (6)	0.019 (7)	0.015 (7)
F2'	0.082 (10)	0.101 (11)	0.067 (8)	−0.024 (8)	0.039 (7)	0.009 (7)
F3'	0.102 (11)	0.073 (9)	0.094 (10)	0.033 (8)	0.039 (8)	0.015 (7)
F4'	0.100 (12)	0.111 (12)	0.134 (13)	−0.018 (9)	0.052 (9)	0.002 (9)
F5'	0.114 (12)	0.101 (12)	0.116 (12)	0.033 (9)	0.021 (9)	−0.005 (9)
F6'	0.037 (8)	0.083 (11)	0.033 (9)	−0.009 (7)	0.032 (7)	0.002 (7)
N1	0.0253 (10)	0.0285 (11)	0.0319 (11)	0.0030 (8)	0.0105 (8)	0.0018 (8)
N2	0.0319 (11)	0.0288 (11)	0.0321 (11)	−0.0008 (9)	0.0165 (9)	−0.0039 (9)
N3	0.0322 (11)	0.0332 (11)	0.0325 (11)	0.0028 (9)	0.0130 (9)	−0.0019 (9)
O1	0.0328 (10)	0.0339 (10)	0.0514 (12)	0.0035 (8)	0.0113 (9)	−0.0043 (9)
C1	0.0380 (14)	0.0310 (13)	0.0274 (12)	0.0017 (10)	0.0190 (11)	−0.0021 (10)
C2	0.0354 (13)	0.0364 (14)	0.0305 (13)	0.0051 (11)	0.0174 (11)	−0.0016 (11)
C3	0.0335 (13)	0.0269 (12)	0.0314 (13)	0.0033 (10)	0.0124 (10)	0.0017 (10)
C4	0.0318 (14)	0.0500 (17)	0.0410 (15)	0.0025 (12)	0.0159 (12)	−0.0058 (13)
C5	0.0377 (14)	0.0323 (14)	0.0337 (13)	0.0018 (11)	0.0166 (11)	−0.0033 (10)
C6	0.0378 (15)	0.0461 (17)	0.0433 (15)	−0.0078 (12)	0.0210 (12)	−0.0107 (13)
C7	0.0544 (18)	0.0345 (14)	0.0419 (15)	−0.0075 (12)	0.0270 (14)	−0.0057 (12)
C8	0.0418 (14)	0.0340 (14)	0.0323 (13)	−0.0042 (11)	0.0215 (11)	−0.0052 (11)
C9	0.0391 (14)	0.0381 (15)	0.0357 (14)	0.0082 (11)	0.0195 (12)	0.0039 (11)
C10	0.0421 (15)	0.0278 (13)	0.0478 (16)	−0.0030 (11)	0.0193 (13)	0.0012 (12)
C11	0.0483 (16)	0.0335 (14)	0.0420 (15)	0.0088 (12)	0.0190 (13)	0.0016 (12)

C12	0.0465 (16)	0.0276 (13)	0.0471 (16)	0.0012 (11)	0.0183 (13)	−0.0052 (12)
C13	0.0627 (19)	0.0275 (13)	0.0463 (16)	0.0018 (13)	0.0271 (15)	0.0005 (12)
C14	0.0552 (18)	0.0516 (18)	0.0409 (16)	0.0011 (14)	0.0290 (14)	−0.0024 (13)
C15	0.0341 (16)	0.051 (2)	0.084 (3)	0.0072 (14)	0.0059 (16)	−0.0075 (18)

Geometric parameters (Å, °)

P1—F1'	1.534 (8)	C2—C4	1.409 (4)
P1—F4'	1.539 (8)	C2—C9	1.510 (4)
P1—F6	1.555 (4)	C3—H3	0.9300
P1—F3'	1.563 (8)	C4—C6	1.367 (4)
P1—F3	1.568 (3)	C4—H4	0.9300
P1—F2	1.576 (2)	C5—C11	1.374 (4)
P1—F5'	1.584 (8)	C6—C8	1.409 (4)
P1—F4	1.587 (3)	C6—H6	0.9300
P1—F5	1.589 (3)	C7—C13	1.358 (5)
P1—F1	1.601 (4)	C7—C8	1.420 (4)
P1—F2'	1.616 (8)	C7—H7	0.9300
P1—F6'	1.639 (8)	C9—H9A	0.9700
N1—C3	1.322 (3)	C9—H9B	0.9700
N1—C10	1.380 (3)	C10—C12	1.343 (4)
N1—C9	1.478 (3)	C10—H10	0.9300
N2—C2	1.323 (3)	C11—C13	1.411 (4)
N2—C1	1.362 (3)	C11—H11	0.9300
N2—H2	0.8600	C12—H12	0.9300
N3—C3	1.324 (3)	C13—H13	0.9300
N3—C12	1.369 (4)	C14—H14A	0.9600
N3—C14	1.464 (3)	C14—H14B	0.9600
O1—C5	1.366 (3)	C14—H14C	0.9600
O1—C15	1.436 (4)	C15—H15A	0.9600
C1—C8	1.423 (4)	C15—H15B	0.9600
C1—C5	1.429 (4)	C15—H15C	0.9600
F1'—P1—F4'	94.7 (6)	C10—N1—C9	124.7 (2)
F1'—P1—F6	174.1 (6)	C2—N2—C1	118.2 (2)
F4'—P1—F6	91.2 (7)	C2—N2—H2	120.9
F1'—P1—F3'	93.6 (5)	C1—N2—H2	120.9
F4'—P1—F3'	92.0 (6)	C3—N3—C12	108.3 (2)
F6—P1—F3'	87.0 (7)	C3—N3—C14	125.2 (2)
F1'—P1—F3	85.3 (6)	C12—N3—C14	126.5 (2)
F4'—P1—F3	143.4 (8)	C5—O1—C15	117.5 (2)
F6—P1—F3	90.5 (2)	N2—C1—C8	122.6 (2)
F3'—P1—F3	51.7 (7)	N2—C1—C5	118.8 (2)
F1'—P1—F2	84.7 (6)	C8—C1—C5	118.6 (2)
F4'—P1—F2	125.7 (8)	N2—C2—C4	123.3 (3)
F6—P1—F2	91.3 (2)	N2—C2—C9	116.2 (2)
F3'—P1—F2	142.3 (7)	C4—C2—C9	120.5 (2)
F3—P1—F2	90.74 (19)	N1—C3—N3	109.0 (2)
F1'—P1—F5'	91.8 (5)	N1—C3—H3	125.5
F4'—P1—F5'	90.9 (6)	N3—C3—H3	125.5

F6—P1—F5'	87.3 (7)	C6—C4—C2	118.9 (3)
F3'—P1—F5'	173.7 (7)	C6—C4—H4	120.5
F3—P1—F5'	125.7 (8)	C2—C4—H4	120.5
F1'—P1—F4	91.4 (6)	O1—C5—C11	125.0 (3)
F4'—P1—F4	53.1 (8)	O1—C5—C1	114.9 (2)
F6—P1—F4	92.7 (3)	C11—C5—C1	120.1 (3)
F3—P1—F4	90.3 (2)	C4—C6—C8	120.0 (3)
F2—P1—F4	175.85 (18)	C4—C6—H6	120.0
F5'—P1—F4	144.0 (8)	C8—C6—H6	120.0
F1'—P1—F5	92.1 (6)	C13—C7—C8	119.5 (3)
F6—P1—F5	92.2 (2)	C13—C7—H7	120.2
F3'—P1—F5	128.4 (7)	C8—C7—H7	120.2
F3—P1—F5	177.34 (19)	C6—C8—C7	123.0 (3)
F2—P1—F5	89.34 (17)	C6—C8—C1	117.0 (3)
F5'—P1—F5	54.7 (8)	C7—C8—C1	119.9 (3)
F4—P1—F5	89.4 (2)	N1—C9—C2	112.1 (2)
F4'—P1—F1	89.2 (7)	N1—C9—H9A	109.2
F6—P1—F1	179.5 (3)	C2—C9—H9A	109.2
F3'—P1—F1	93.3 (6)	N1—C9—H9B	109.2
F3—P1—F1	89.4 (2)	C2—C9—H9B	109.2
F2—P1—F1	88.2 (2)	H9A—C9—H9B	107.9
F5'—P1—F1	92.4 (7)	C12—C10—N1	106.7 (2)
F4—P1—F1	87.8 (2)	C12—C10—H10	126.6
F5—P1—F1	88.0 (2)	N1—C10—H10	126.6
F1'—P1—F2'	91.4 (5)	C5—C11—C13	120.2 (3)
F4'—P1—F2'	173.8 (6)	C5—C11—H11	119.9
F6—P1—F2'	82.7 (6)	C13—C11—H11	119.9
F3'—P1—F2'	88.6 (5)	C10—C12—N3	107.6 (2)
F2—P1—F2'	53.8 (7)	C10—C12—H12	126.2
F5'—P1—F2'	87.9 (5)	N3—C12—H12	126.2
F4—P1—F2'	127.9 (7)	C7—C13—C11	121.7 (3)
F5—P1—F2'	142.5 (7)	C7—C13—H13	119.2
F1—P1—F2'	96.9 (6)	C11—C13—H13	119.2
F1'—P1—F6'	176.4 (6)	N3—C14—H14A	109.5
F4'—P1—F6'	88.6 (5)	N3—C14—H14B	109.5
F3'—P1—F6'	87.8 (5)	H14A—C14—H14B	109.5
F3—P1—F6'	93.0 (5)	N3—C14—H14C	109.5
F2—P1—F6'	92.2 (6)	H14A—C14—H14C	109.5
F5'—P1—F6'	86.6 (5)	H14B—C14—H14C	109.5
F4—P1—F6'	91.8 (6)	O1—C15—H15A	109.5
F5—P1—F6'	89.6 (5)	O1—C15—H15B	109.5
F1—P1—F6'	177.5 (6)	H15A—C15—H15B	109.5
F2'—P1—F6'	85.3 (5)	O1—C15—H15C	109.5
C3—N1—C10	108.4 (2)	H15A—C15—H15C	109.5
C3—N1—C9	126.7 (2)	H15B—C15—H15C	109.5
C2—N2—C1—C8	−0.2 (3)	C13—C7—C8—C6	−179.8 (3)
C2—N2—C1—C5	179.5 (2)	C13—C7—C8—C1	0.1 (4)
C1—N2—C2—C4	0.9 (4)	N2—C1—C8—C6	−0.7 (4)
C1—N2—C2—C9	−179.0 (2)	C5—C1—C8—C6	179.6 (2)

C10—N1—C3—N3	−0.8 (3)	N2—C1—C8—C7	179.4 (2)
C9—N1—C3—N3	−175.3 (2)	C5—C1—C8—C7	−0.2 (4)
C12—N3—C3—N1	0.6 (3)	C3—N1—C9—C2	−16.9 (4)
C14—N3—C3—N1	177.7 (2)	C10—N1—C9—C2	169.4 (2)
N2—C2—C4—C6	−0.7 (4)	N2—C2—C9—N1	−93.1 (3)
C9—C2—C4—C6	179.3 (2)	C4—C2—C9—N1	87.0 (3)
C15—O1—C5—C11	1.4 (4)	C3—N1—C10—C12	0.7 (3)
C15—O1—C5—C1	−178.8 (3)	C9—N1—C10—C12	175.4 (2)
N2—C1—C5—O1	0.8 (3)	O1—C5—C11—C13	179.5 (2)
C8—C1—C5—O1	−179.4 (2)	C1—C5—C11—C13	−0.2 (4)
N2—C1—C5—C11	−179.4 (2)	N1—C10—C12—N3	−0.4 (3)
C8—C1—C5—C11	0.3 (4)	C3—N3—C12—C10	−0.1 (3)
C2—C4—C6—C8	−0.3 (4)	C14—N3—C12—C10	−177.2 (3)
C4—C6—C8—C7	−179.2 (3)	C8—C7—C13—C11	0.1 (4)
C4—C6—C8—C1	0.9 (4)	C5—C11—C13—C7	0.0 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···F1^{i}	0.93	2.46	3.204 (5)	137
C9—H9A···F2^{ii}	0.97	2.49	3.244 (4)	135
C3—H3···O1^{iii}	0.93	2.27	3.122 (3)	152

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

Fig. 1

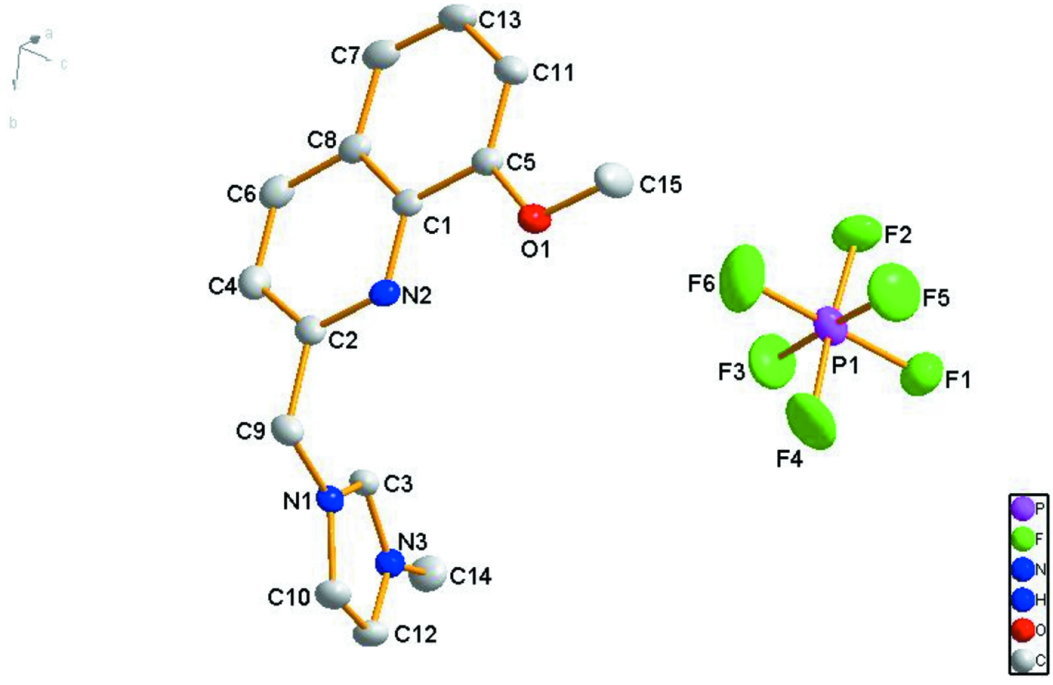
C13
C7
C11
C8
C5
C15
C6
C1
O1
C4
N2
C2
C9
N1
C3
N3
C14
C10
C12
F2
F6
F5
F3
P1
F1
F4
P
F
N
H
O
C

Fig. 2