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2-(2,4-Dimethylphenyl)-4-isopropyl-1-methylisoquinolinium hexafluorophosphate

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Key indicators

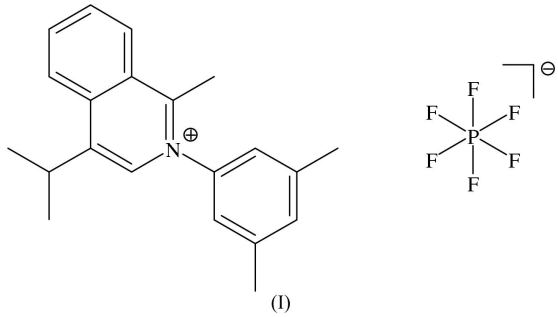
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.124
Data-to-parameter ratio = 14.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{21}H_{24}N^+\cdot PF_6^-$, crystallizes in centrosymmetric hydrogen-bonded clusters consisting of two cations and two anions, *via* weak aromatic C—H···F interactions. The isoquinolinium and dimethylphenyl moieties are not coplanar.

Comment

In the context of the study of ring-closure reactions with imines (Diederen *et al.*, 1998), the crystal structure of the title reaction product, (I), was determined. The title compound crystallizes in the triclinic space group $P\overline{1}$ and features hydrogen-bonded cation/anion pairs, which are related by the centre of symmetry. These pairs are joined by weak aromatic C—H···F hydrogen bonds, between H5 and F4^{i} [symmetry code: (i) $1-x, 1-y, -z$; 2.51 Å], and between H19 and F6^{ii} [symmetry code: (ii) $1+x, y, z$; 2.53 Å]. These hydrogen bonds are in the 2.1–2.6 Å region reported for C—H···F(P) interactions (Grepioni *et al.*, 1998), and are likely to be the reason that the PF_6^- anion is not disordered in this case.



(I)

The isoquinolinium ring system and the 2,4-dimethylphenyl group are not coplanar, probably because of unfavourable steric interactions between H19 and the H atoms on C10, resulting in a dihedral angle of 71.58 (8)° between their least-squares planes.

Experimental

The compound was synthesized by J. Diederen (University of Amsterdam), and recrystallized from dichloromethane and pentane.

Crystal data

$C_{21}H_{24}N^+\cdot PF_6^-$
M_r = 435.38
Triclinic, $P\overline{1}$
a = 8.7413 (4) Å
b = 9.0199 (5) Å
c = 12.8984 (5) Å
α = 93.027 (3)°
β = 98.039 (3)°
γ = 90.032 (2)°
V = 1005.55 (8) Å^3
Z = 2
D_x = 1.438 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9057 reflections
θ = 1.6–26.0°
μ = 0.20 mm^{-1}
T = 150 (2) K
Block, colourless
0.2 × 0.14 × 0.11 mm

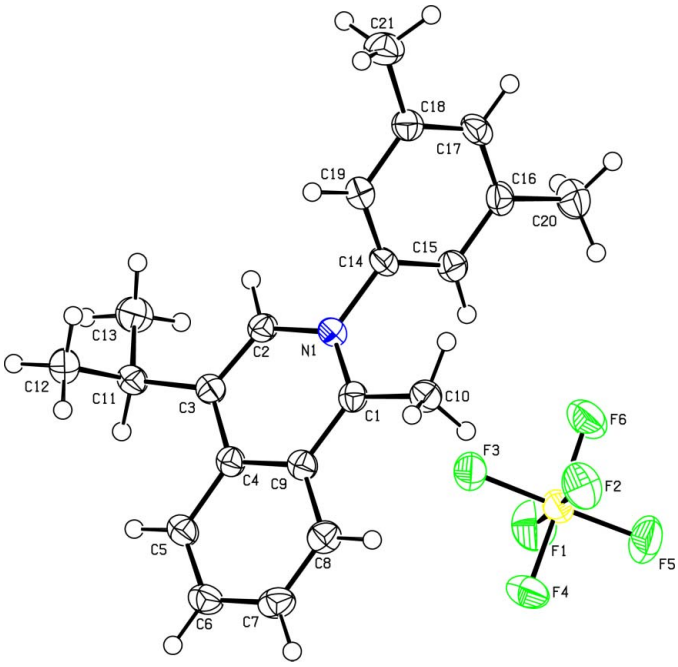


Figure 1
View of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*MULABS*; Blessing, 1995)
T_{min} = 0.80, T_{max} = 0.97
9057 measured reflections
3931 independent reflections
2547 reflections with $I > 2\sigma(I)$
R_{int} = 0.063
θ_{max} = 26.0°
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 9$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.124
S = 0.99
3931 reflections
267 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0614P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···F4^{i}	0.95	2.51	3.445 (2)	167
C19—H19···F6^{ii}	0.95	2.53	3.384 (3)	149

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $x+1, y, z$.

All H atoms were placed in geometrically idealized positions (C—H = 0.95–1.00 Å) and constrained to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and U_{iso}(H) = 1.2U_{eq}(C) for all other H atoms.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *HKL2000* (Otwinowski & Minor, 1997); data reduction: *HKL2000*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

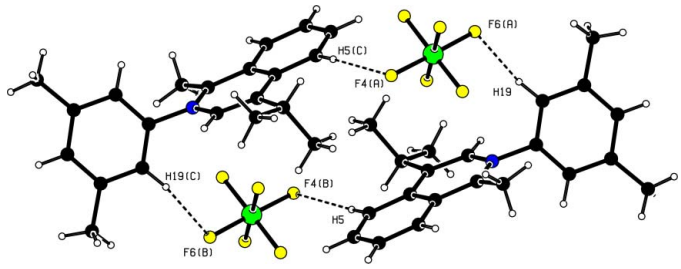


Figure 2
Hydrogen-bonded (dashed lines) centrosymmetric cluster of two cations and two anions. [Symmetry codes: (*A*) $1+x, y, z$; (*B*) $1-x, 1-y, -z$; (*C*) $2-x, 1-y, -z$.]

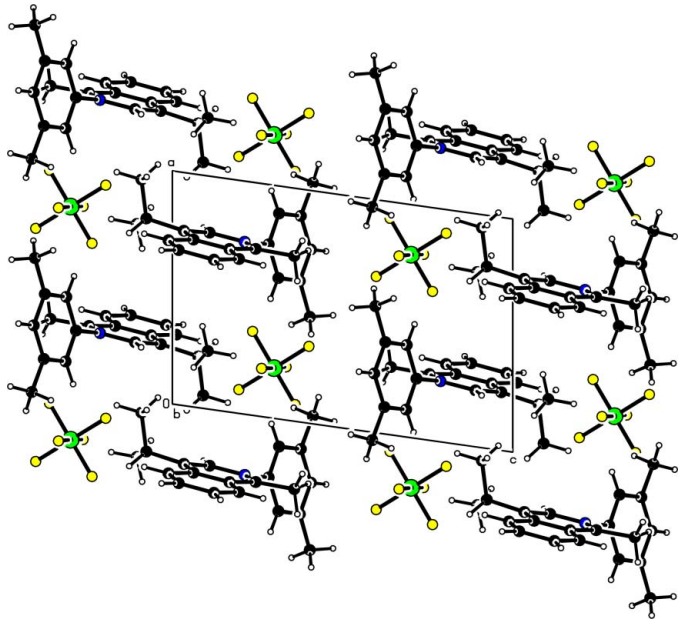


Figure 3
Packing diagram. View along the crystallographic *b* axis.

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