

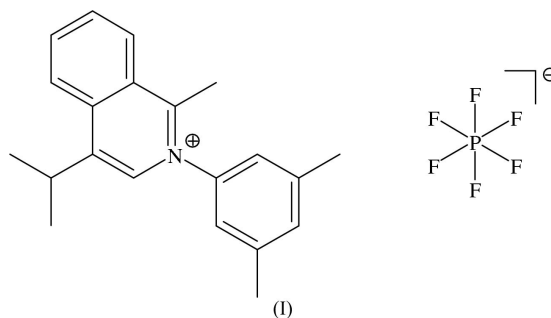
2-(2,4-Dimethylphenyl)-4-isopropyl-1-methyl-
isoquinolinium hexafluorophosphateDuncan M. Tooke,* Martin Lutz
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Key indicators

Single-crystal X-ray study
 $T = 150$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.048
 wR factor = 0.124
Data-to-parameter ratio = 14.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.The title compound, $\text{C}_{21}\text{H}_{24}\text{N}^+\cdot\text{PF}_6^-$, crystallizes in centrosymmetric hydrogen-bonded clusters consisting of two cations and two anions, *via* weak aromatic $\text{C}-\text{H}\cdots\text{F}$ interactions. The isoquinolinium and dimethylphenyl moieties are not coplanar.

Comment

In the context of the study of ring-closure reactions with imines (Diederer *et al.*, 1998), the crystal structure of the title reaction product, (I), was determined. The title compound crystallizes in the triclinic space group $P\bar{1}$ and features hydrogen-bonded cation/anion pairs, which are related by the centre of symmetry. These pairs are joined by weak aromatic $\text{C}-\text{H}\cdots\text{F}$ hydrogen bonds, between H5 and F4ⁱ [symmetry code: (i) $1-x, 1-y, -z$; 2.51 Å], and between H19 and F6ⁱⁱ [symmetry code: (ii) $1+x, y, z$; 2.53 Å]. These hydrogen bonds are in the 2.1–2.6 Å region reported for $\text{C}-\text{H}\cdots\text{F}(\text{P})$ interactions (Grepioni *et al.*, 1998), and are likely to be the reason that the PF_6^- anion is not disordered in this case.

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. Diederer (University of Amsterdam), and recrystallized from dichloromethane and pentane.

Crystal data

 $\text{C}_{21}\text{H}_{24}\text{N}^+\cdot\text{PF}_6^-$
 $M_r = 435.38$
Triclinic, $P\bar{1}$
 $a = 8.7413$ (4) Å
 $b = 9.0199$ (5) Å
 $c = 12.8984$ (5) Å
 $\alpha = 93.027$ (3)°
 $\beta = 98.039$ (3)°
 $\gamma = 90.032$ (2)°
 $V = 1005.55$ (8) Å³ $Z = 2$
 $D_x = 1.438$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 9057
reflections
 $\theta = 1.6$ – 26.0 °
 $\mu = 0.20$ mm⁻¹
 $T = 150$ (2) K
Block, colourless
 $0.2 \times 0.14 \times 0.11$ mm

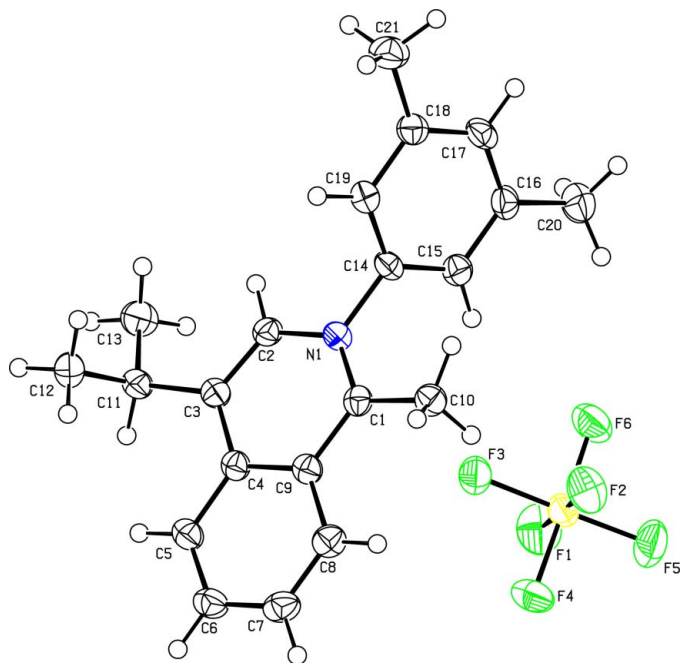


Figure 1
View of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Data collection

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

Refinement

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

Table 1

Hydrogen-bond geometry ($\text{Å}, ^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C5-H5 \cdots F4^i$	0.95	2.51	3.445 (2)	167
$C19-H19 \cdots F6^{ii}$	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 ($C-H = 0.95-1.00 \text{ Å}$) 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*.

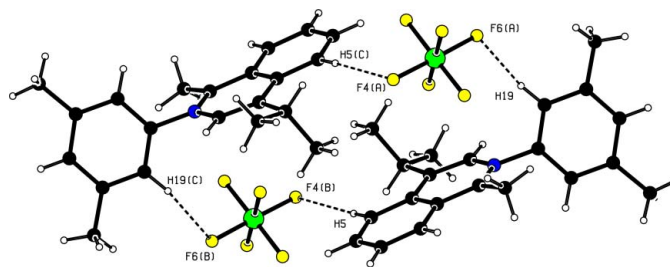


Figure 2
Hydrogen-bonded (dashed lines) centrosymmetric cluster of two cations and two anions. [Symmetry codes: (A) $1 + x, y, z$; (B) $1 - x, 1 - y, -z$; (C) $2 - x, 1 - y, -z$.]

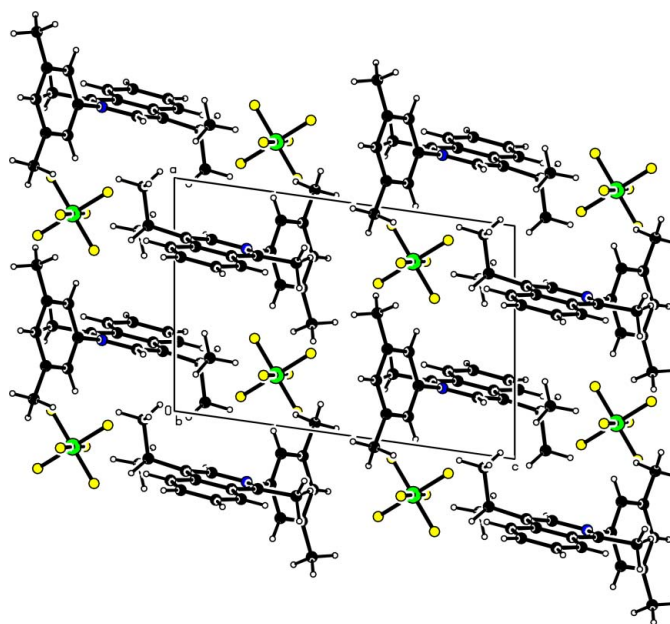


Figure 3
Packing diagram. View along the crystallographic b axis.

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