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3-Methyl-1-(morpholinocarbonylmethyl)-imidazolium hexafluorophosphate

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.063
wR factor = 0.152
Data-to-parameter ratio = 17.0

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

In the title compound, $C_{10}H_{16}N_3O_2^+\cdot PF_6^-$, the morpholine ring adopts a chair conformation and the methylimidazole and morpholine rings are *anti* to one another.

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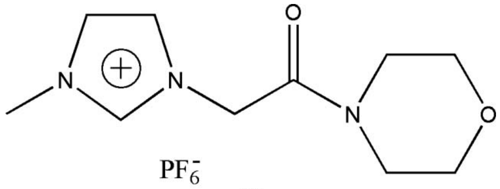
Comment

The title salt, (I), is an ionic compound which was obtained in the synthesis of amide-functionalized imidazolium ionic liquids. These liquids, first reported by Gathergood *et al.* (2004), are biodegradable ionic liquids whose function is thought to be related to the amide-functionalized group in the alkyl side chain.



(I)

The structure of (I) is shown in Fig. 1. The morpholine ring exhibits a normal chair conformation. The N1—C1—C6—N2 torsion angle of 177.8 (2)° indicates that the imidazole and morpholine rings are *anti* to one another. Atoms C1, C6, N2 and O2 are essentially coplanar [O2—C1—C6—N2 = −0.7 (3)°]. The dihedral angles between this plane and the plane of the five-membered ring and the plane through atoms C2, C3, C4 and C5 are 82.66 (1)° and 55.79 (1)°, respectively.

Experimental

The title compound was prepared according to the procedures of Speziale *et al.* (1956) and Gathergood *et al.* (2004). Suitable crystals

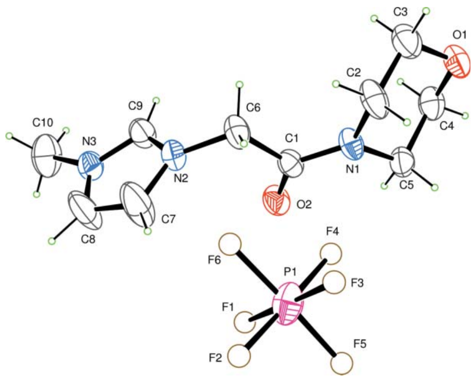


Figure 1
View of (I), showing 40% probability displacement ellipsoids. H atoms are drawn as spheres of arbitrary radii.

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were obtained by slow evaporation of an acetone solution at room temperature (m.p. 411–413 K).

Crystal data

$C_{10}H_{16}N_3O_2^+\cdot PF_6^-$
$M_r = 355.22$
Monoclinic, $P2_1/c$
$a = 13.075$ (4) Å
$b = 9.682$ (4) Å
$c = 11.888$ (4) Å
$\beta = 99.134$ (18)°
$V = 1485.9$ (9) Å^3
$Z = 4$
$D_x = 1.588$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.26$ mm^{-1}
$T = 296$ (1) K
Chunk, colorless
0.55 × 0.47 × 0.42 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.863$, $T_{\max} = 0.896$
14263 measured reflections
3393 independent reflections
2334 reflections with $F^2 > 2\sigma(F^2)$
$R_{\rm int} = 0.034$
$\theta_{\max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.152$
$S = 1.01$
3393 reflections
200 parameters
H-atom parameters constrained
$w = 1/[0.0005F_o^2 + 5\sigma(F_o^2)]/(4F_o^2)$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.59$ e Å^{-3}
$\Delta\rho_{\min} = -0.50$ e Å^{-3}
Extinction correction: Larson (1970)
Extinction coefficient: 6.5 (6) × 10^2

All H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and refined using a riding model, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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