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Key indicators

Single-crystal X-ray study
 $T = 153\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
Disorder in solvent or counterion
 R factor = 0.036
 wR factor = 0.099
Data-to-parameter ratio = 16.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.1-Benzyl-3-[4-(dibromomethyl)benzyl]imidazolium
hexafluorophosphate

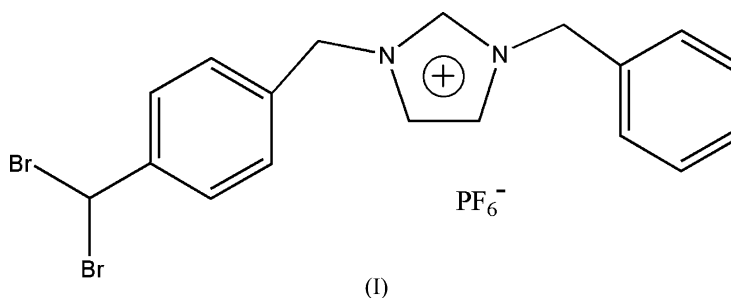
In the crystal structure of the title compound, $\text{C}_{18}\text{H}_{17}\text{Br}_2\text{N}_2^+\cdot\text{PF}_6^-$, four F atoms of the hexafluorophosphate anion are disordered. The hexafluorophosphate ions are linked to 1-benzyl-3-[4-(dibromomethyl)benzyl]imidazolium cations by $\text{C}-\text{H}\cdots\text{F}$ hydrogen bonds, which may be effective in the stabilization of the crystal structure.

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Comment

Numerous flexible and rigid *N*-heterocyclic carbene precursors have been synthesized and studied. They have attracted considerable attention due to their diverse coordination capabilities and the important catalytic properties of their metal complexes (Herrmann, 2002; Herrmann & Kocher, 1997). We here report the crystal structure of the title compound, (I).



In the structure of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings *A* (atoms C1–C6), *B* (N1/N2/C8–C10) and *C* (C12–C17) are, of course, planar; the dihedral angles between them are $A/B = 68.94(3)^\circ$, $A/C = 29.64(3)^\circ$ and $B/C = 64.76(3)^\circ$.

As can be seen from the packing diagram (Fig. 2), the hexafluorophosphate molecules are linked to 1-benzyl-3-[4-(dibromomethyl)benzyl]imidazolium by $\text{C}-\text{H}\cdots\text{F}$ hydrogen bonds (Table 1), which may be effective in the stabilization of the crystal structure. Dipole–dipole and van der Waals interactions are also effective in the molecular packing.

Experimental

The title compound was synthesized by the reaction of 1-(bromomethyl)-4-(dibromomethyl)benzene with 1-benzyl-1*H*-imidazole in tetrahydrofuran at 350 K, according to a literature method (Lee *et al.*, 2004). The resulting white deposit was dissolved in methanol (20 ml) and then ammonium hexafluorophosphate (2 g) was added. The white solid was filtered off, washed with diethyl ether and air-dried. White single crystals suitable for X-ray diffraction were obtained by recrystallization from absolute acetonitrile and diethyl ether (1:2).

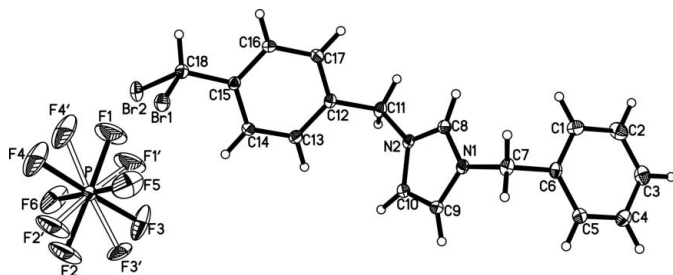


Figure 1

The asymmetric unit of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Both disorder components are shown.

Crystal data

$C_{18}H_{17}Br_2N_2^+ \cdot PF_6^-$

$M_r = 566.13$

Monoclinic, $P2_1/c$

$a = 9.9544$ (2) Å

$b = 14.2182$ (3) Å

$c = 14.2552$ (3) Å

$\beta = 91.963$ (1)°

$V = 2016.41$ (7) Å³

$Z = 4$

$D_x = 1.865$ Mg m⁻³

Mo $K\alpha$ radiation

$\mu = 4.16$ mm⁻¹

$T = 153$ (2) K

Block, white

$0.51 \times 0.47 \times 0.44$ mm

Data collection

Rigaku R-AXIS RAPID
diffractometer

ω scans

Absorption correction: multi-scan
(Blessing, 1995)

$T_{\min} = 0.138$, $T_{\max} = 0.160$

19223 measured reflections

4610 independent reflections

4042 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.049$

$\theta_{\max} = 27.5^\circ$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.099$

$S = 1.01$

4610 reflections

282 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 1.96P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.84$ e Å⁻³

$\Delta\rho_{\min} = -0.74$ e Å⁻³

Extinction correction: *SHELXL97*

Extinction coefficient: 0.0095 (7)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C8-H8 \cdots F2^i$	0.95	2.52	3.016 (4)	113
$C9-H9 \cdots F3^{ii}$	0.95	2.51	3.297 (5)	141
$C11-H11A \cdots F6^{iii}$	0.99	2.38	3.288 (4)	152
$C18-H18 \cdots F6^{iv}$	1.00	2.47	3.273 (4)	137

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

Four F atoms of the hexafluorophosphate were found to be disordered, with refined site occupancies of 0.851 (4) and 0.149 (4). H

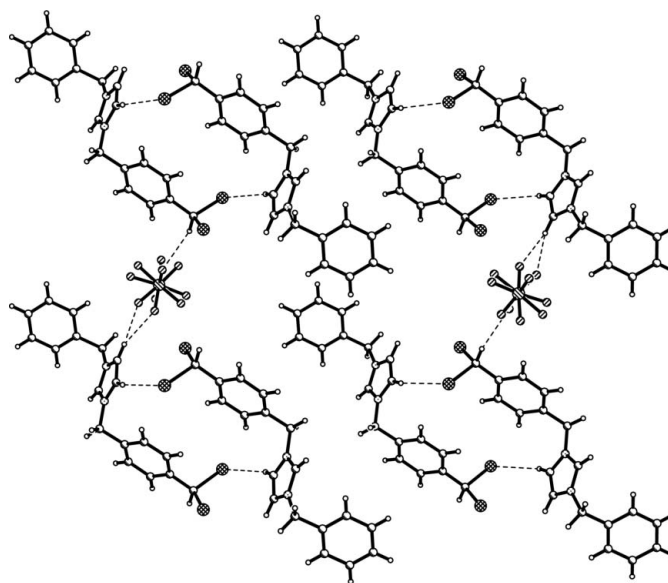


Figure 2

A packing diagram of (I). Hydrogen bonds are shown as dashed lines. Both disorder components are shown.

atoms were positioned geometrically, with $C-H = 0.95, 1.00$ and 0.99 Å for aromatic, methine and methylene H atoms, respectively, and constrained to ride on their parent atoms, with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$.

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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