

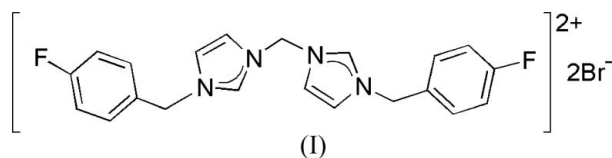
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Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.009\text{ \AA}$
 R factor = 0.047
 wR factor = 0.123
Data-to-parameter ratio = 19.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.1,1'-Bis(4-fluorobenzyl)-3,3'-methylene-
diimidazolium dibromideIn the title structure, $\text{C}_{21}\text{H}_{20}\text{F}_2\text{N}_4^{2+}\cdot 2\text{Br}^-$, the central C atom of the cation is located on a crystallographic twofold rotation axis. The dihedral angle between the imidazole rings is $75.50(17)^\circ$.

Comment

Our group is currently interested in transition metal complexes of chelating *N*-heterocyclic carbene (NHC) ligands. These ligands can be typically derived from imidazolium salts. In our previous work (Lee *et al.*, 2004), we reported several bis(imidazolium) salts and their corresponding bidentate palladium bis(NHC) complexes. Among them was the Pd complex of 1,1'-bis(4-fluorobenzyl)-3,3'-methylenediimidazolium dibromide. We report here the crystal structure of the free ligand, (I).The molecular structure of (I) is shown in Fig. 1. The central C atom lies on a twofold rotation axis. The structure is very similar to the analogous structures bearing a 4-methoxybenzyl (Lee *et al.*, 2004) and a 3-methoxybenzyl substituent (Lee & Chiu, 2004). In (I), the dihedral angle between the two methylene-linked imidazole rings is $75.50(17)^\circ$, comparable to the angle of $78.02(7)^\circ$ reported for the 3-methoxybenzyl analog (Lee & Chiu, 2004).

Experimental

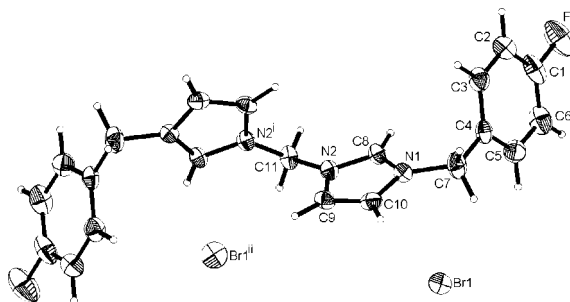
The title compound was prepared according to a literature procedure (Lee *et al.*, 2004). Crystals were obtained by slow diffusion of diethyl ether into a dimethylformamide solution of (I).

Figure 1

The molecular structure of (I), showing 35% displacement ellipsoids for non-H atoms. [Symmetry codes: (i) $-x, y, \frac{1}{2} - z$; (ii) $1 - x, 1 - y, 1 - z$.]

Crystal data

$C_{21}H_{20}F_2N_4^{2+} \cdot 2Br^-$
 $M_r = 526.23$
 Monoclinic, $C2/c$
 $a = 33.465$ (11) Å
 $b = 5.375$ (2) Å
 $c = 12.077$ (4) Å
 $\beta = 104.93$ (1)°
 $V = 2099.0$ (13) Å³

$Z = 4$
 $D_x = 1.664$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 3.89$ mm⁻¹
 $T = 298$ (2) K
 Parallelepiped, colorless
 $0.34 \times 0.20 \times 0.18$ mm

Data collection

Bruker SMART 1000
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 2002)
 $T_{\min} = 0.351$, $T_{\max} = 0.496$

6381 measured reflections
 2506 independent reflections
 1339 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.069$
 $\theta_{\text{max}} = 28.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.123$
 $S = 0.98$
 2506 reflections
 132 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0473P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.58$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.40$ e Å⁻³

All H atoms were placed in calculated positions, with C–H = 0.95–0.99 Å, and included in the riding-model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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References

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