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## Key indicators

Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$   
Disorder in solvent or counterion  
 $R$  factor = 0.073  
 $wR$  factor = 0.236  
Data-to-parameter ratio = 11.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## 1-(9-Anthracenylmethyl)-3-butylbenzimidazolium hexafluorophosphate

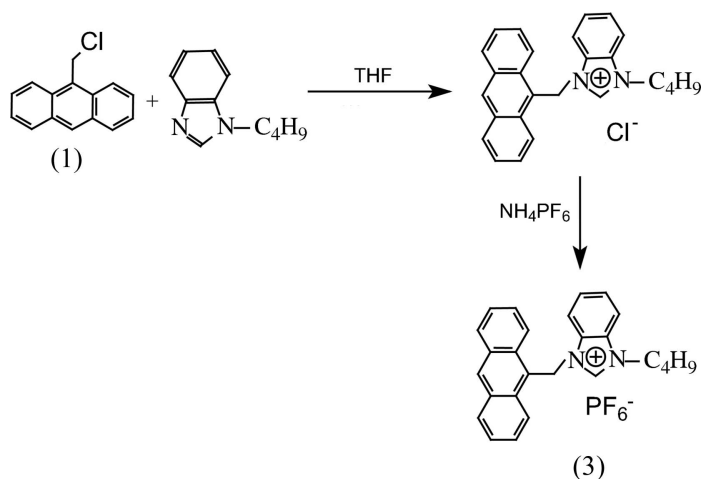
In the title compound,  $\text{C}_{26}\text{H}_{25}\text{N}_2^+\cdot\text{PF}_6^-$ , the dihedral angle between the anthracene and benzimidazole ring systems is  $93.8(1)^\circ$ . The anthracenylmethyl and butyl units lie on opposite sides of the benzimidazole ring system.

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## Comment

After the isolation of free stable imidazol-2-ylidene (Imy) (Arduengo *et al.*, 1991), metal carbenes based on the imidazole ring have attracted considerable attention, owing to their inherent stability, their interesting characteristics of structure and bonding, and their potential for synthesis and as catalysts in organic reactions (Fischer *et al.*, 2006). We report here the synthesis and crystal structure of 1-(9-anthracenylmethyl)-3-butylbenzimidazolium hexafluorophosphate, (3). 9-Chloromethylanthracene, (1), reacted with 1-butylbenzimidazole to afford a yellow powder, 1-(9-anthracenylmethyl)-3-butylbenzimidazolium chloride, (2). Compound (2) and  $\text{NH}_4\text{PF}_6$  undergo an anionic exchange reaction to give compound (3). Crystals of (3) suitable for X-ray diffraction were obtained by evaporating slowly a  $\text{CH}_2\text{Cl}_2$  solution at room temperature. In (3), the anthracenylmethyl and butyl units lie on opposite sides of the benzimidazole ring system, and the dihedral angle between the anthracene and benzimidazole ring systems is  $93.8(1)^\circ$  (Fig. 1). The N1–C21, N1–C22, N2–C16 and N2–C22 bond distances [1.394 (4), 1.335 (4), 1.408 (4) and 1.310 (4) Å, respectively] are similar to those [1.379 (7), 1.335 (7), 1.334 (8) and 1.331 (8) Å] observed in 1-(9-anthracenylmethyl)-3-ethylimidazolium iodide (Liu *et al.*, 2003). The N2–C22–N1 bond angle is  $111.1(3)^\circ$ , which is somewhat larger than that [ $108.8(6)^\circ$ ] found in 1-(9-anthracenylmethyl)-3-ethylimidazolium iodide.



## Experimental

A solution of 1-butylbenzimidazole (6.840 g, 0.039 mol) and 9-chloromethylantracene (8.480 g, 0.037 mol) in THF (150 ml) was stirred for three days under reflux. The yellow product was filtered and washed with THF. Yellow crystals of (2) were obtained by recrystallization from acetone/diethyl ether (yield 12.80 g, 85%). M.p. 512–514 K.  $\text{NH}_4\text{PF}_6$  (12.773 g, 0.0784 mol) was added to a methanol solution (150 ml) of (2) (8.038 g, 0.020 mol). A yellow precipitate formed immediately, which was collected by filtration, washed with small portions of methanol and dried in a vacuum to give (3) as a yellow powder (yield 9.820 g, 96%). M.p. 489–491. Analysis calculated for  $\text{C}_{26}\text{H}_{25}\text{F}_6\text{N}_2\text{P}$ : C 61.18, H 4.94, N 5.49, P 6.07, F 22.33%; found: C 60.92, H 4.57, N 5.62, P 6.36, F 22.58%.

### Crystal data

|   |   |
|---|---|
| $\text{C}_{26}\text{H}_{25}\text{N}_2^+\text{PF}_6^-$ | $V = 1212.3 (12) \text{ \AA}^3$           |
| $M_r = 510.45$  | $Z = 2$                                   |
| Triclinic, $P\bar{1}$                                 | $D_x = 1.398 \text{ Mg m}^{-3}$           |
| $a = 9.568 (5) \text{ \AA}$                           | Mo $K\alpha$ radiation                    |
| $b = 11.818 (7) \text{ \AA}$                          | $\mu = 0.18 \text{ mm}^{-1}$              |
| $c = 12.523 (7) \text{ \AA}$                          | $T = 293 (2) \text{ K}$                   |
| $\alpha = 112.956 (8)^\circ$                          | Prism, yellow                             |
| $\beta = 109.260 (8)^\circ$                           | $0.22 \times 0.18 \times 0.16 \text{ mm}$ |
| $\gamma = 91.257 (8)^\circ$                           |   |

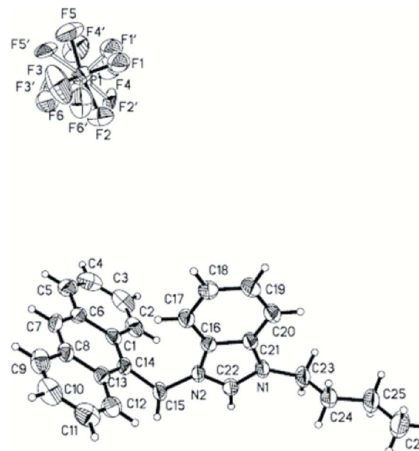
### Data collection

|   |  |
|---|--|
| Bruker SMART CCD area-detector diffractometer               | 6505 measured reflections              |
| $\varphi$ and $\omega$ scans                                | 4200 independent reflections           |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | 2271 reflections with $I > 2\sigma(I)$ |
| $T_{\min} = 0.962$ , $T_{\max} = 0.972$                     | $R_{\text{int}} = 0.043$               |
|   | $\theta_{\max} = 25.0^\circ$           |

### Refinement

|                                 |  |
|---------------------------------|--|
| Refinement on $F^2$             | $w = 1/[\sigma^2(F_o^2) + (0.1446P)^2]$        |
| $R[F^2 > 2\sigma(F^2)] = 0.073$ | where $P = (F_o^2 + 2F_c^2)/3$                 |
| $wR(F^2) = 0.236$               | $(\Delta/\sigma)_{\max} < 0.001$               |
| $S = 0.98$                      | $\Delta\rho_{\max} = 0.42 \text{ e \AA}^{-3}$  |
| 4200 reflections                | $\Delta\rho_{\min} = -0.32 \text{ e \AA}^{-3}$ |
| 370 parameters                  | Extinction correction: SHELXL97                |
| H-atom parameters constrained   | Extinction coefficient: 0.006 (4)              |

All H atoms were initially located in a difference Fourier map and were then placed in geometrically idealized positions and constrained to ride on their parent atoms with C–H distances in the range 0.93–0.97 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  [ $1.5U_{\text{eq}}(\text{C})$  for methyl atoms]. The hexafluorophosphate ion is disordered over two positions and these were refined with anisotropic displacement parameters and with P–F



**Figure 1**

A view of (3) along with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

distances restrained to 1.58 (5) Å. The occupancy factors are 0.677 (4) and 0.323 (4), respectively.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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