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Tetra-*n*-butylammonium tetrakis(pentafluorophenyl)borate

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.005 Å
R factor = 0.033
wR factor = 0.075
Data-to-parameter ratio = 6.9

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

In the title compound, $C_{16}H_{36}N^+\cdot C_{24}BF_{20}^-$, the geometric parameters do not show any unusual values. The four *n*-butyl chains adopt an all-*trans* conformation.

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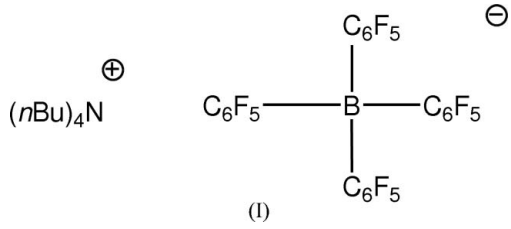
Comment

Very strong cationic Lewis acids are only available in the presence of weakly coordinating counter-ions such as $[B(C_6F_5)_4]^-$. These anions also play an important role in electrochemistry. The salt $[^nBu_4N]^+\cdot[B(C_6F_5)_4]^-$ possesses a low reactivity towards reducing and oxidizing agents. Moreover, conductance measurements show that the dissociation constants of $[^nBu_4N]^+\cdot[B(C_6F_5)_4]^-$ solutions in solvents with low polarity are greater than those of smaller traditional anions (LeSuer *et al.*, 2004). Therefore, we are convinced that tetra-*n*-butylammonium tetrakis(pentafluorophenyl)borate, (I), is an ideal supporting electrolyte. We have synthesized (I) and we report its crystal structure here.



(I)

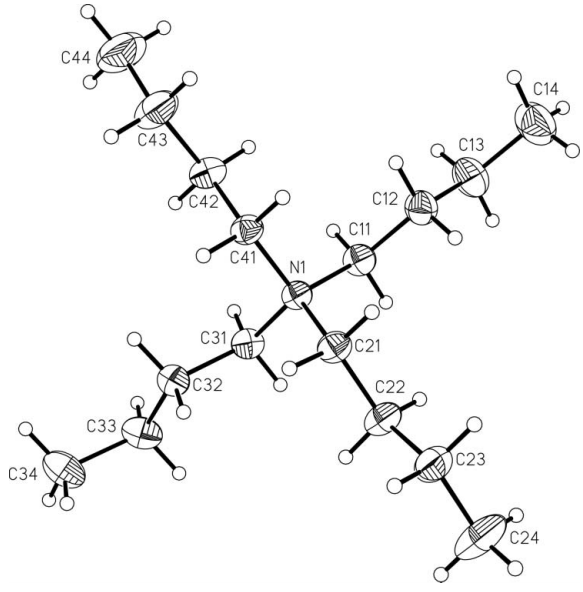


Figure 1
Perspective view of the cation of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Perspective views of the cation and anion of (I) are shown in Figs. 1 and 2, respectively. Bond lengths and angles can be regarded as normal (Cambridge Crystallographic Database; Version 1.6 plus three updates; Mogul Version 1.0; Allen, 2002). The four *n*-butyl chains adopt an all-*trans* conformation.

Experimental

Compound (I) was synthesized according to the literature procedure of LeSuer *et al.* (2004). Colourless crystals of the title compound suitable for X-ray diffraction were grown from a methanol solution at 253 K.

Crystal data

$C_{16}H_{36}N^+\cdot C_{24}BF_{20}^-$	D_x = 1.480 Mg m^{-3}
M_r = 921.51	Mo $K\alpha$ radiation
Monoclinic, *Cc*	Cell parameters from 10062 reflections
a = 24.104 (2) Å	θ = 3.6–25.6°
b = 12.8925 (12) Å	μ = 0.15 mm^{-1}
c = 17.5363 (15) Å	T = 173 (2) K
β = 130.629 (5)°	Block, colourless
V = 4135.9 (7) Å^3	0.42 × 0.37 × 0.21 mm
Z = 4	

Data collection

Stoe IPDS-II two-circle diffractometer	3371 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.035
Absorption correction: none	θ_{max} = 25.6°
10176 measured reflections	$h = -29 \rightarrow 29$
3854 independent reflections	$k = -15 \rightarrow 14$
	$l = -21 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.033	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.075	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
S = 1.00	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
3854 reflections	Extinction correction: *SHELXL97*
560 parameters	Extinction coefficient: 0.0036 (4)
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

N1—C11	1.527 (4)	B1—C81	1.657 (4)
N1—C31	1.528 (4)	B1—C51	1.660 (5)
N1—C41	1.529 (3)	B1—C71	1.666 (4)
N1—C21	1.529 (3)	B1—C61	1.681 (4)

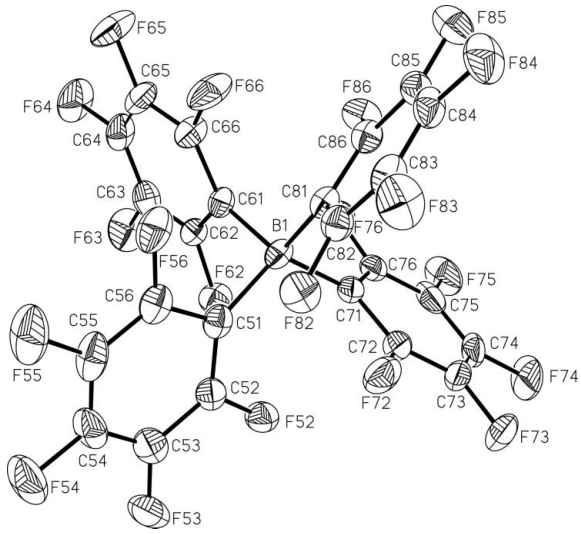


Figure 2
Perspective view of the anion of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

H atoms were located in a difference map, but refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}($C_{methylene}$) or U_{iso}(H) = 1.5U_{eq}(C_{methyl})] using a riding model, with C—H = 0.98 and 0.99 Å for C_{methyl} and $C_{methylene}$, respectively. In the absence of significant anomalous scatterers, Friedel pairs were merged.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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