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Tetra-*n*-butylammonium hexafluorophosphate

Frauke Schödel, Hans-Wolfram Lerner and Michael Bolte*

Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Marie-Curie-Straße 11, 60439 Frankfurt/Main, Germany

Correspondence e-mail:
bolte@chemie.uni-frankfurt.de

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The structure of the title compound, $C_{16}H_{36}N^+\cdot PF_6^-$, has been reported previously by Angaridis, Cotton & Petrukhina [*Inorg. Chim. Acta* (2001), **324**, 318–323]. However, these authors found the PF_6^- ion to be heavily disordered and they did not publish any coordinates. We present here a redetermination of this structure, based on new intensity data and exhibiting no disorder.

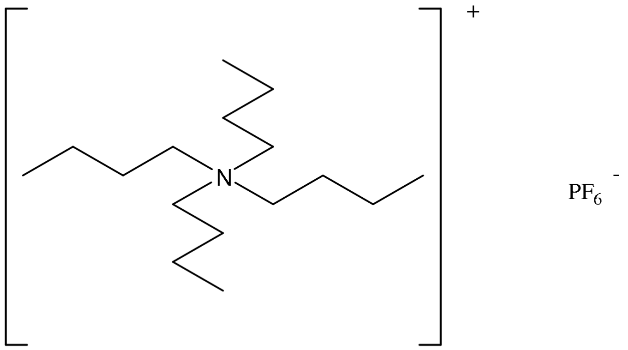
Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.005 Å
R factor = 0.057
wR factor = 0.159
Data-to-parameter ratio = 15.6

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

Comment

A perspective view of the title compound, (I), is shown in Fig. 1. The structure is composed of discrete $[C_{16}H_{36}N]^+$ cations and PF_6^- anions. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 1.6 plus three updates; *MOGUL* Version 1.0; Allen, 2002). Just one C—C—C—C torsion angle deviates from an antiperiplanar conformation [C41—C42—C43—C44 = 71.0 (4)°]; the other three angles are close to 180°. Since no coordinates from the previously published structure determination of this compound (Angaridis *et al.*, 2001) are available, no comparison between the two structure determinations can be made.



(I)

Experimental

X-ray quality crystals of (I) were obtained on recrystallization from CH_2Cl_2 at ambient temperature.

Crystal data

$C_{16}H_{36}N^+\cdot PF_6^-$
M_r = 387.43
Monoclinic, $P2_1/c$
a = 9.4057 (19) Å
b = 13.593 (2) Å
c = 14.982 (3) Å
β = 91.367 (16)°
V = 1914.9 (6) Å^3
Z = 4
D_x = 1.344 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7863 reflections
θ = 2.6–24.8°
μ = 0.20 mm^{-1}
T = 173 (2) K
Rod, colourless
0.29 × 0.14 × 0.12 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: none
13397 measured reflections
3379 independent reflections

1764 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.081$
$\theta_{\rm max} = 25.0°$
$h = -11 \rightarrow 11$
$k = -16 \rightarrow 16$
$l = -17 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.159$
$S = 0.91$
3379 reflections
217 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0896P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.50$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.49$ e Å^{-3}

H atoms were refined with fixed individual displacement parameters [$U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) or 1.5$U_{\rm eq}$(C$_{\rm methyl}$)], using a riding model, with C—H = 0.99 and 0.98 Å for methyleme and methyl H atoms, respectively.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2003).

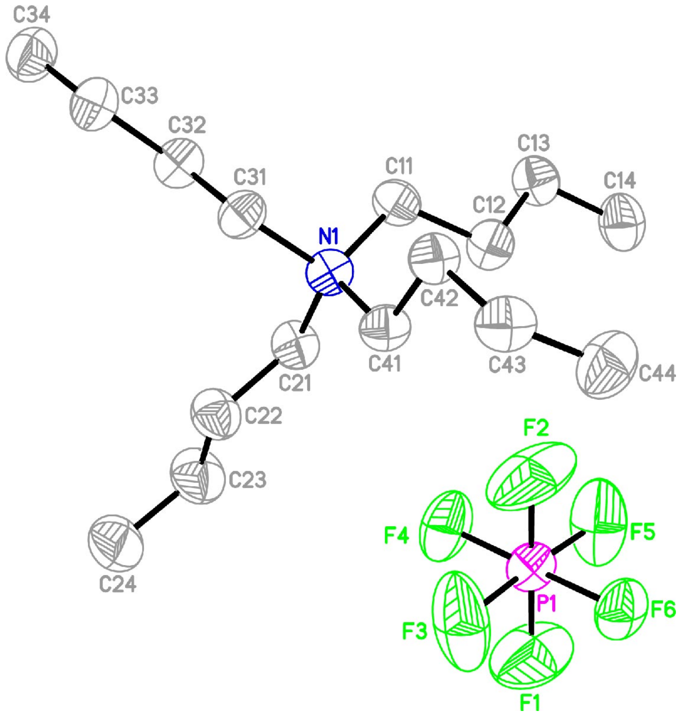


Figure 1
Perspective view of the title compound, with the atom numbering; displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity.

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