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Key indicators

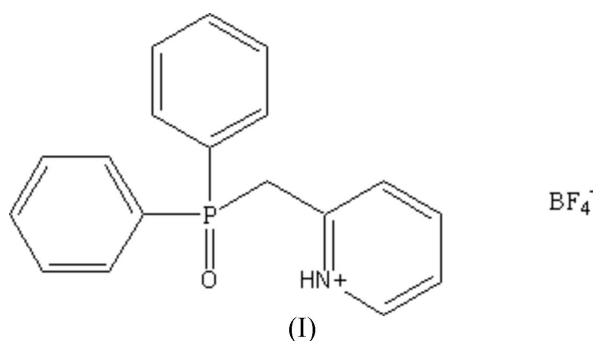
Single-crystal X-ray study
 $T = 110$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.049
 wR factor = 0.138
Data-to-parameter ratio = 19.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.2-(Diphenylphosphino)ethylpyridinium
tetrafluoroborate

In the title compound, $[\text{OPPh}_2(2\text{-CH}_2\text{C}_5\text{H}_4\text{NH})]\text{BF}_4$, the phosphorus atom displays a tetrahedral geometry, with the nitrogen of the pyridyl group protonated and having tetrafluoroborate as counter-anion.

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Comment

Vapor diffusion of diethyl ether into a solution reaction of $\text{Cu}(\text{BF}_4)_2$ with 2-pyridyldiphenylphosphine in acetonitrile at 278 K, provided two easily distinguished kinds of crystals: blue block-shaped crystals corresponding to the reaction product of the Cu^{II} salt with the bidentate phosphine ligand and colorless block-shaped crystals of the title compound, (I). An X-ray crystallographic investigation showed (I) to be the oxidized ligand, with further protonation of the nitrogen of the pyridyl group (Fig. 1) due to the presence of water in the system, the charge being balanced by BF_4^- present in the solution. The so-called hemilabile hybrid ligand (Minghetti *et al.*, 1998) presents a very close to tetrahedral geometry, with the angles around the P atom ranging from $105.61(8)$ to $112.31(7)^\circ$ (Table 1). The bond lengths and angles are in normal ranges (Allen *et al.*, 1987).



In the crystal structure, the molecules are linked into two chains running in different directions (Fig. 2) by $\text{C}-\text{H} \cdots \text{F}$ and $\text{N}-\text{H} \cdots \text{O}$ intermolecular hydrogen bonds (Table 2).

Experimental

The title compound, (I), was obtained from the oxidation and protonation of 2-pyridyldiphenylphosphine from a reaction solution containing $\text{Cu}(\text{BF}_4)_2$ (0.102 g, 0.4 mmol); the phosphine ligand (0.110 g, 0.4 mmol) was synthesized as reported in the literature with slight modifications of the procedure (Akermark *et al.*, 1986). Diffraction-quality crystals of (I) were obtained by vapor diffusion of diethyl ether into a concentrated acetonitrile solution of the reaction mixture in the presence of air.

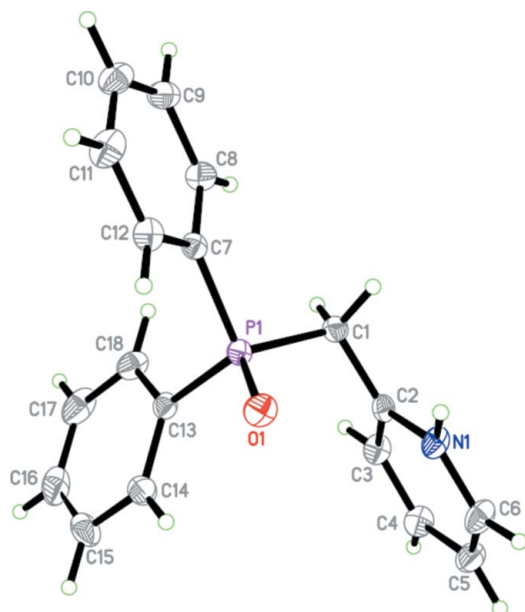


Figure 1
A view of the molecular structure of the cation of (I), with displacement ellipsoids drawn at the 50% probability level

Crystal data

$C_{18}H_{17}NOP^+ \cdot BF_4^-$
 $M_r = 381.11$
 Monoclinic, $C2/c$
 $a = 16.7528$ (15) Å
 $b = 13.9287$ (17) Å
 $c = 15.661$ (2) Å
 $\beta = 95.314$ (4)°
 $V = 3638.7$ (7) Å³

$Z = 8$
 $D_x = 1.391$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.20$ mm⁻¹
 $T = 110$ (2) K
 Block, colorless
 $0.29 \times 0.25 \times 0.21$ mm

Data collection

Bruker APEX X8 CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS, Bruker, 2000)
 $T_{\min} = 0.958$, $T_{\max} = 0.960$

14958 measured reflections
 4726 independent reflections
 3915 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.041$
 $\theta_{\text{max}} = 29.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.138$
 $S = 1.04$
 4726 reflections
 239 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0684P)^2 + 4.7739P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.65$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.57$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

P1—O1	1.4939 (12)	P1—C13	1.8000 (17)
P1—C7	1.7946 (17)	P1—C1	1.8283 (18)
O1—P1—C7	112.31 (7)	O1—P1—C1	111.51 (8)
O1—P1—C13	110.04 (8)	C7—P1—C1	105.61 (8)
C7—P1—C13	108.97 (8)	C13—P1—C1	108.22 (8)

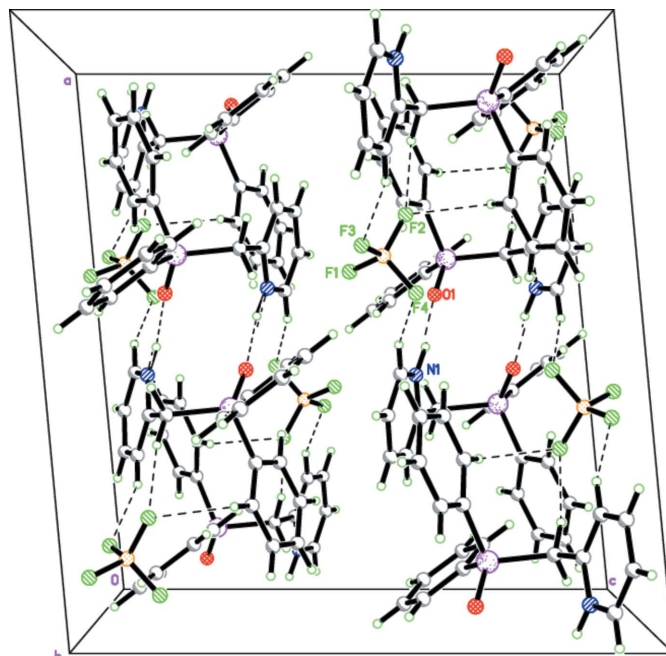


Figure 2
Packing diagram of (I), showing the C—H...F and N—H...O hydrogen bonds as dashed lines.

Table 2

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
N1—H1C...O1 ⁱ	0.96 (3)	1.67 (3)	2.6212 (18)	169 (2)
C1—H1A...F2 ⁱⁱ	0.99	2.38	3.356 (2)	169
C18—H18...F2 ⁱⁱ	0.95	2.49	3.265 (3)	139
C3—H3...F3 ⁱⁱⁱ	0.95	2.46	3.345 (2)	155
C6—H6...F4 ⁱⁱⁱ	0.95	2.40	3.271 (3)	152

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

The H atom attached to the N atom was located in a difference map and refined isotropically. All other H atoms were positioned geometrically, with C—H = 0.95 or 0.99 Å for aromatic and methylene H atoms, respectively, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *APEX2* (Bruker, 2003); cell refinement: *APEX2*; data reduction: *SAINT-Plus* (Bruker, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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