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(4,7-Diphenyl-1,10-phenanthroline)bis(triphenylphosphine)copper(I) tetrafluoroborate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.136
Data-to-parameter ratio = 15.8

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

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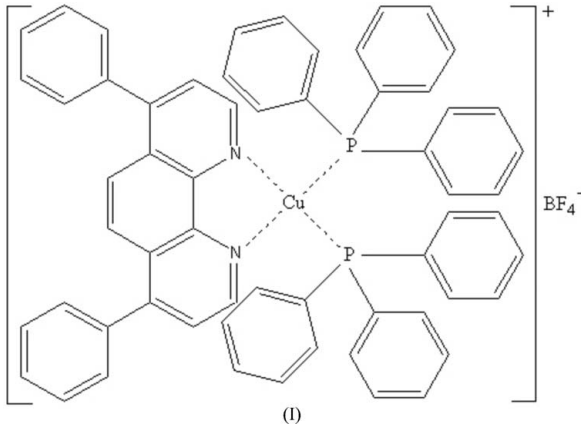
The title compound, $[Cu(C_{24}H_{16}N_2)(C_{18}H_{15}P)_2]BF_4$, consists of mononuclear $Cu(PPh_3)_2(NN)^+$ and BF_4^- ions (NN is 4,7-diphenyl-1,10-phenanthroline). The Cu^I atom is four-coordinated by two P atoms of PPh_3 groups and two N donors of two NN ligands to form a tetrahedral coordination geometry.

Comment

It is well known that the mixed-ligand complexes of the $Cu(PPh_3)_2(NN)^+$ cation, where PPh_3 and NN denote triphenylphosphine and 4,7-diphenyl-1,10-phenanthroline, respectively, both exhibit strong phosphorescent emissions in the solid state at room temperature. These Cu^I complexes have been investigated for a long time, with regard to their preparation (Kirchhoff *et al.*, 1985), photophysical properties (Palmer *et al.*, 1987) and so on. However, reports on the crystal structures of complexes with 4,7-diphenyl-1,10-phenanthroline or its derivatives are rare (Chesnut *et al.*, 2001). We report here the crystal structure of a 4,7-diphenyl-1,10-phenanthroline Cu^I complex, (I).



(I)

The title compound, $Cu(PPh_3)_2(NN)^+\cdot BF_4^-$, consists of mononuclear $Cu(PPh_3)_2(NN)^+$ and BF_4^- ions. The Cu^I atom is four-coordinated by two P atoms of distinct PPh_3 groups and two N donors of derivatives of 1,10-phenanthroline, to form a tetrahedral coordination geometry (Fig. 1). Selected geometric parameters are given in given in Table 1.

Experimental

Complex (I) was synthesized according to the method of Cuttell *et al.* (2002). A mixture of $[Cu(NCCH_3)_4]BF_4$ (310.0 mg, 1.0 mmol) and triphenylphosphine (524.6 mg, 2.0 mmol) in CH_2Cl_2 (30 ml) was stirred at room temperature for 1 h, and then 4,7-diphenyl-1,10-phenanthroline (332.4 mg, 1.0 mmol) was added to the mixture. The

reaction mixture was stirred for an additional 1 h and filtered, and the clear yellow filtrate was concentrated to *ca* 12 ml. Acetonitrile (about 10 ml) was added, and the vapor diffusion of diethyl ether into the resulting solution gave yellow crystals of the complex (80% yield).

Crystal data

$[Cu(C_{24}H_{16}N_2)(C_{18}H_{15}P)_2]BF_4$	D_x = 1.321 Mg m^{-3}
M_r = 1007.28	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 5088 reflections
a = 20.5552 (15) Å	θ = 2.3–25.9°
b = 11.9349 (9) Å	μ = 0.55 mm^{-1}
c = 21.2725 (15) Å	T = 293 (2) K
β = 103.870 (1)°	Plate, yellow
V = 5066.5 (6) Å^3	0.40 × 0.29 × 0.06 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	9962 independent reflections
	7512 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.028
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)	θ_{max} = 26.0°
	$h = -24 \rightarrow 25$
T_{min} = 0.845, T_{max} = 0.966	$k = -14 \rightarrow 11$
27936 measured reflections	$l = -26 \rightarrow 21$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$w = 1/[\sigma^2(F_o^2) + (0.0841P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.136	
S = 1.05	$(\Delta/\sigma)_{max}$ = 0.001
9962 reflections	$\Delta\rho_{max}$ = 0.70 e Å^{-3}
631 parameters	$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—N2	2.0782 (19)	Cu—P2	2.2271 (6)
Cu—N1	2.0802 (17)	Cu—P1	2.2796 (7)
N2—Cu—N1	80.14 (7)	N2—Cu—P1	108.34 (5)
N2—Cu—P2	119.88 (5)	N1—Cu—P1	101.75 (5)
N1—Cu—P2	122.61 (5)	P2—Cu—P1	117.50 (2)

H atoms were included in calculated positions and treated as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

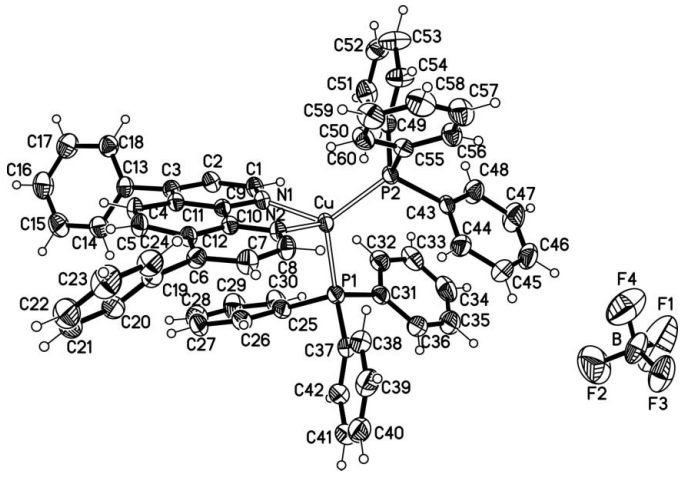


Figure 1
The molecular structure of the title compound, with 30% probability displacement ellipsoids.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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