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(μ-4,4′-Bipyridine-κ^2N:N')bis[(1,10-phenanthroline-κ^2N,N')(triphenylphosphine-κP)copper(I)] bis(tetrafluoroborate)

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Key indicators

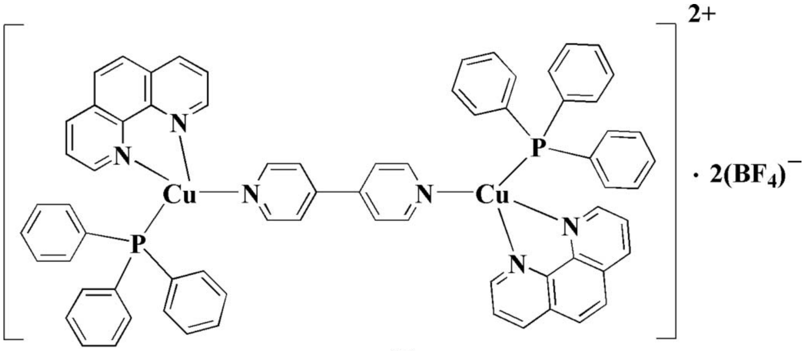
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.058
wR factor = 0.163
Data-to-parameter ratio = 16.1

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

The dinuclear cation in the title compound, $[Cu_2(C_{10}H_8N_2)(C_{12}H_8N_2)_2(C_{18}H_{15}P)_2](BF_4)_2$, lies on a centre of inversion. Each Cu^I atom is coordinated by 1,10-phenanthroline, triphenylphosphine and a bridging 4,4′-bipyridine molecule, and has a distorted tetrahedral coordination geometry. The two Cu^I atoms are displaced by 0.32 (1) Å on either side of the mean plane of the 4,4′-bipyridine unit.

Comment

Complexes of low-valent metals such as Fe^{II}, Ru^{II} or Cu^I with chelating, heteroaromatic ligands such as 1,10-phenanthroline (phen) are an important class of compounds (Blake *et al.*, 1998; Ponganis *et al.*, 1980; Scott *et al.*, 1998). As a result of the presence of low-energy π* orbitals on the phen ligand, the adducts exhibit strong metal–ligand charge-transfer (CT) absorption bands in the visible spectrum. Copper(I) complexes based on polypyridyl ligands are therefore of interest on account of their potential utility in harvesting solar energy (Alonso-Vante *et al.*, 1994). We report here the title complex, (I).



(I)

The structure of the cation in (I) is centrosymmetric (Fig. 1). Each Cu^I atom is coordinated by 1,10-phenanthroline, triphenylphosphine and the bridging 4,4′-bipyridine molecule, and has a distorted tetrahedral coordination geometry (Table 1). The central portion of the molecule is distorted from planarity, with the two Cu^I atoms displaced by 0.32 (1) Å on either side of the mean plane of the 4,4′-bipyridine unit.

Experimental

All reactions were performed under a nitrogen atmosphere. Solvents were distilled using standard techniques and saturated with N_2 prior to use. $[Cu(CH_3CN)_4](BF_4)$ was prepared according to a published method (Kubas *et al.*, 1990). $[Cu(CH_3CN)_4](BF_4)$ (0.0315 g, 0.1 mmol) was added to a solution of 4,4′-bipyridine (0.0078 g, 0.05 mmol) in dichloromethane (30 ml). The mixture was stirred at room temperature for 2 h, then 1,10-phenanthroline (0.018 g, 0.1 mmol) and triphenylphosphine (0.0262 g, 0.1 mmol) were added. Slow diffusion of diethyl ether into the dichloromethane solution yielded brown block-shaped crystals of (I) suitable for X-ray diffraction (yield 70%).

Crystal data

$[Cu_2(C_{10}H_8N_2)(C_{12}H_8N_2)_2$-
$(C_{18}H_{15}P)_2](BF_4)_2$
$M_r = 1341.83$
Monoclinic, $P2_1/n$
$a = 14.192$ (7) Å
$b = 15.372$ (7) Å
$c = 14.515$ (6) Å
$\beta = 92.495$ (9)°

$V = 3164$ (2) Å^3
$Z = 2$
$D_x = 1.409$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.79$ mm^{-1}
$T = 293$ (2) K
Block, brown
0.26 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.850$, $T_{max} = 0.880$

17926 measured reflections
6518 independent reflections
3572 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 26.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.163$
$S = 1.00$
6518 reflections
406 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0746P)^2 + 1.4838P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.78$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.033 (4)	Cu1—N2	2.096 (4)
Cu1—N3	2.060 (3)	Cu1—P1	2.1999 (14)
N1—Cu1—N3	119.04 (14)	N1—Cu1—P1	117.14 (10)
N1—Cu1—N2	81.13 (15)	N3—Cu1—P1	109.56 (10)
N3—Cu1—N2	108.35 (14)	N2—Cu1—P1	119.09 (11)

H atoms were placed in calculated positions, with C—H = 0.93 Å, and allowed to ride during subsequent refinement, with $U_{iso}(H) = 1.2U_{eq}(C)$.

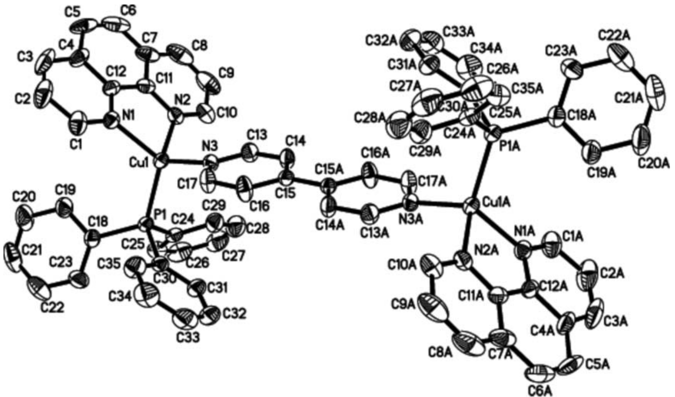


Figure 1
The molecular structure of the cation in (I), showing displacement ellipsoids drawn at the 30% probability level. H atoms are omitted. The suffix A denotes atoms generated by the symmetry operation ($2 - x$, $1 - y$, $1 - z$).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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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