Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

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

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Received 14 November 2006
Accepted 19 November 2006

Key indicators

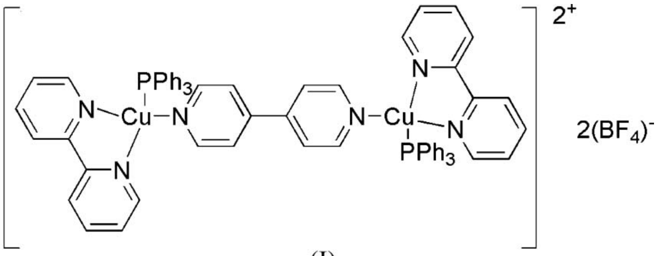
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.008 Å
Disorder in solvent or counterion
R factor = 0.060
wR factor = 0.138
Data-to-parameter ratio = 14.2

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

The new air-stable title complex, $[Cu_2(C_{10}H_8N_2)_3(C_{18}H_{15}P)_2](BF_4)_2$, has been synthesized and characterized by X-ray diffraction. The complex is a centrosymmetric dimer with pairs of Cu^I atoms bridged by 4,4′-bipyridine. In addition to the 4,4′-bipyridine N atom, each Cu^I atom is coordinated by one chelating 2,2′-bipyridine ligand and one triphenylphosphine ligand to give a distorted CuN$_3$P tetrahedral geometry.

Comment

There has been great interest in binuclear polypyridyl complexes because of their interesting photophysical and photochemical properties, and their possible use as potential catalysts, as multi-electron storage systems and in the design of novel functional materials (Kalyanasundaram & Gratzel, 1993; Juris *et al.*, 1988; Meyer, 1986; Rauer *et al.*, 1997). The specific role of the bridging ligands is influenced by the acceptor and donor properties of the coordination sites, the length and rigidity of the spacers, the presence or absence of conjugated bonds, and the orientation of the substituents and the ligand charge. Copper(I) complexes with various N, S, P and halide donor ligands are of growing interest owing to their wide variation in structural format and rich photophysical and photochemical properties. Many of these complexes have been reported to be luminescent with emission behavior that varies with structure, the identity of halides, and steric and electronic effects of the ligands (Yam *et al.*, 1996; Yam & Lo, 1999; Simon *et al.*, 1996; Su *et al.*, 1997; Li *et al.*, 2005; Wu *et al.*, 2005).



(I)

The structure of the $[Cu_2(C_{10}H_8N_2)(C_{10}H_8N_2)_2(C_{18}H_{15}P)_2]$ cation in the title compound, (I), is shown in Fig. 1, and selected bond lengths and angles are given in Table 1. The complex is a centrosymmetric dimer with pairs of Cu^I atoms bridged by 4,4′-bipyridine. The Cu^I center has a distorted tetrahedral geometry. All the Cu—N bond distances are essentially identical to those found in the literature (Zhou *et al.*, 2006; Chandra *et al.*, 2002). Similar results were obtained for the Cu—P bond distances.

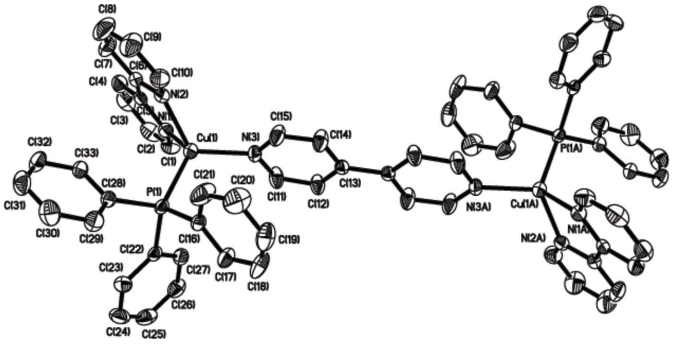


Figure 1
The molecular structure of the cation of (I). Displacement ellipsoids are shown at the 30% probability level. H atoms have been omitted. [Symmetry code: (A) $-x + 1, -y + 1, -z + 1$.]

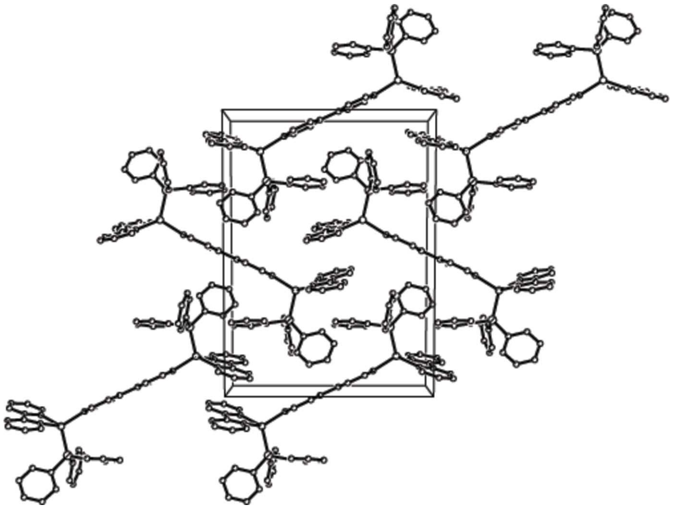


Figure 2
The packing of (I). H atoms and anions have been omitted.

Experimental

To a CH_2Cl_2 (30 ml) solution of 4,4′-bipyridine (15.6 mg, 0.10 mmol) under an atmosphere of N_2 was added $[Cu(CH_3CN)_4]BF_4$ (63.0 mg, 0.20 mmol) to give a red solution. After the solution was stirred at room temperature for 2 h, 2,2′-bipyridine (21.2 mg, 0.20 mmol) was added, and after another 4 h, triphenylphosphine (52.4 mg, 0.2 mmol). Recrystallization by slow diffusion of diethyl ether into the CH_2Cl_2 solution gave brown crystals suitable for X-ray diffraction (yield 0.091 g, 57%).

Crystal data

$[Cu_2(C_{10}H_8N_2)_3(C_{18}H_{15}P)_2](BF_4)_2$
$M_r = 1293.79$
Monoclinic, $P2_1/c$
$a = 10.010\ (11)$ Å
$b = 14.723\ (17)$ Å
$c = 20.21\ (2)$ Å
$\beta = 98.716\ (19)°$
$V = 2944\ (6)$ Å^3
$Z = 2$
$D_x = 1.460$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.85$ mm^{-1}
$T = 292\ (2)$ K
Block, brown
$0.20 \times 0.14 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.889$, $T_{max} = 0.9$
16611 measured reflections
6015 independent reflections
3672 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 26.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.138$
$S = 1.03$
6015 reflections
425 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 1.3321P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N3	2.030 (4)	Cu1—N2	2.057 (4)
Cu1—N1	2.050 (4)	Cu1—P1	2.206 (3)
N3—Cu1—N1	118.01 (16)	N3—Cu1—P1	109.62 (12)
N3—Cu1—N2	116.33 (14)	N1—Cu1—P1	120.51 (10)
N1—Cu1—N2	79.97 (16)	N2—Cu1—P1	109.14 (11)

All H atoms were placed in calculated positions. The H atoms were then constrained to an ideal geometry with C–H distances of 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The fluorine atoms are disordered over two sites, with site occupancy factors which refined to 0.655 (10) and 0.345 (10). F···F distances were restrained to 2.30 (2) and B···F to 1.37 (1).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000; 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, 2000); software used to prepare material for publication: *SHELXTL*.

We are grateful to the State Key Project (No. 2005CCA06800) for financial support. We thank the foundation (50418010) for NSFC/RGC Joint Research.

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