Bis[μ-bis(diphenylphosphino)methane-$\kappa^2P:P'$]-bis[(1,10-phenanthroline-κ^2N,N')copper(I)] bis(tetrafluoroborate) dichloromethane disolvate

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In the structure of the title complex, $[Cu_2(C_{25}H_{22}P_2)_2(C_{12}H_8N_2)_2](BF_4)_2\cdot2CH_2Cl_2$, the two Cu centres are bridged by two bis(diphenylphosphino)methane (dppm) ligands to form a centrosymmetric eight-membered $Cu_2P_4C_2$ ring. The coordination of polyhedron of each Cu atom is distorted tetrahedral.

Comment

The four-electron-donor diphosphine ligand, bis(diphenylphosphino)methane (dppm), is a very efficient bridging bidentate ligand and can form polynuclear complexes with most metal ions (Puddephatt, 1983; Morton & Orpen, 1992). Copper(I) complexes with dppm have received the most attention, due to their diverse coordination geometry and rich photophysical properties (Jitendra *et al.*, 1999; Yam *et al.*, 2001). Here, we report the preparation and crystal structure determination of the title compound, (I), a new dinuclear copper(I) complex with dppm.

(I)
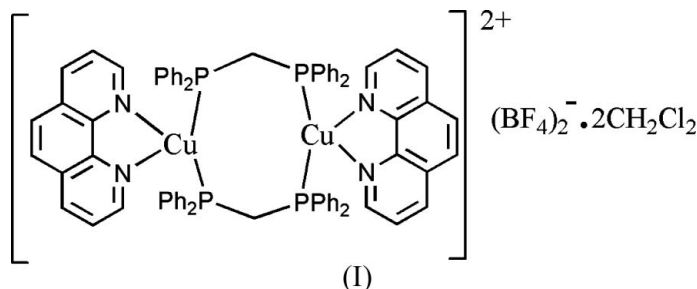
The molecular structure of (I) is illustrated in Fig. 1, and selected bond distances and angles are given in Table 1. Compound (I) consists of a centrosymmetric dimer of $[Cu(phen)(dppm)]^+$ cations (phen is 1,10-phenanthroline), tetrafluoroborate anions and solvent dichloromethane molecules. The two Cu centres are bridged by two dppm ligands to form a centrosymmetric eight-membered $Cu_2P_4C_2$ ring. The remaining coordination sites on each Cu atom are occupied by two N atoms of a phen ligand. The Cu^I atoms adopt a distorted tetrahedral coordination geometry, with the angles around the Cu atoms ranging from 79.2 (2)° for N1—Cu1—N2 to 133.33 (8)° for P1—Cu1—P2A (the suffix A denotes the symmetry position $2-x$, $-y$, $-z$).

Compound (I) can be regarded as similar to $[Cu2(\mu_2\text{-}dppm)_2(phen)_2](PF_6)_2\cdot2(CH_3COCH_3)$ (Kitagawa *et al.*, 1991). The Cu—N and Cu—P bond distance are within the normal ranges (Cao *et al.*, 2005) and similar to those in the above-mentioned complex. The Cu···Cu separation of 4.720 (5) Å is shorter than that in the trinuclear complexes $[Cu_3(dppm)_3(\mu_3\text{-}X)_2]^+$ (X is Cl, Br and I; Jitendra *et al.*, 1999).
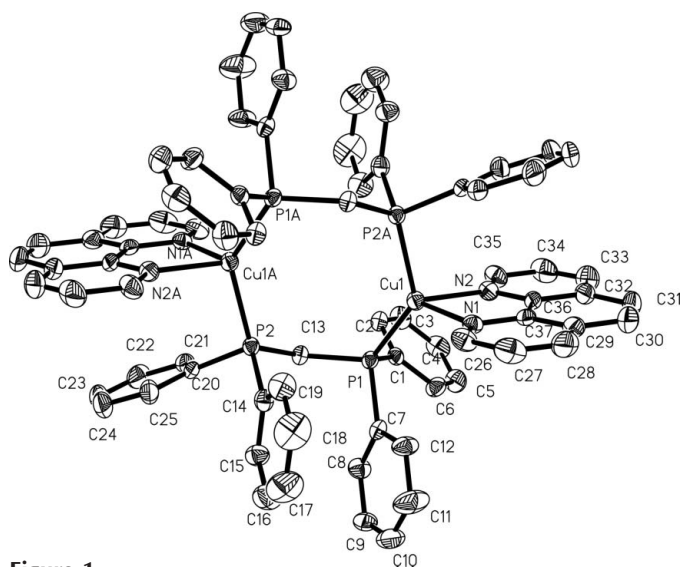
Figure 1
The molecular structure of compound (I), showing the atom-numbering scheme and with displacement ellipsoids drawn at the 30% probability level. H atoms, the tetrafluoroborate anions and solvent dichloromethane molecules have been omitted for clarity. [Symmetry code: (A) $2-x$, $-y$, $-z$]

Experimental

Reaction of equimolar amounts of $[Cu(CH_3CN)_4]BF_4$, phen and dppm in dichloromethane under a dinitrogen atmosphere gave an orange solution. Yellow crystals of (I), suitable for X-ray diffraction analysis, were obtained by vapour diffusion of diethyl ether into the dichloromethane solution.

Crystal data

$[Cu_2(C_{25}H_{22}P_2)_2(C_{12}H_8N_2)_2]$- $(BF_4)_2 \cdot 2CH_2Cl_2$	$Z = 1$
$M_r = 1599.69$	$D_x = 1.453$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 11.318$ (5) Å	Cell parameters from 703
$b = 12.461$ (5) Å	reflections
$c = 14.710$ (6) Å	$\theta = 2.7$–$24.2°$
$\alpha = 104.177$ (7)°	$\mu = 0.88$ mm^{-1}
$\beta = 103.851$ (7)°	$T = 293$ (2) K
$\gamma = 105.822$ (7)°	Block, yellow
$V = 1827.8$ (13) Å^3	$0.20 \times 0.16 \times 0.14$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	6403 independent reflections
	3689 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.048$
Absorption correction: multi-scan ($SADABS$; Sheldrick, 1996)	$\theta_{max} = 25.0°$
	$h = -13 \rightarrow 13$
$T_{min} = 0.738$, $T_{max} = 0.884$	$k = -14 \rightarrow 14$
9428 measured reflections	$l = -17 \rightarrow 13$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.077$	$w = 1/[\sigma^2(F_o^2) + (0.0856P)^2]$
$wR(F^2) = 0.197$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.001$
6403 reflections	$\Delta\rho_{max} = 0.66$ e Å^{-3}
515 parameters	$\Delta\rho_{min} = -0.52$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.111 (5)	Cu1—P1	2.231 (2)
Cu1—N2	2.124 (5)	Cu1—P2^i	2.269 (2)
N1—Cu1—N2	79.2 (2)	N1—Cu1—P2^i	98.91 (15)
N1—Cu1—P1	121.60 (15)	N2—Cu1—P2^i	102.78 (15)
N2—Cu1—P1	106.47 (16)	P1—Cu1—P2^i	133.33 (8)

Symmetry codes: (i) $-x + 2$, $-y$, $-z$.

All H atoms were positioned geometrically and treated as riding atoms, with C—H bond distances in the range 0.93–0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$. The tetrafluoroborate anion and solvent dichloromethane molecules are disordered, with occupanices of 0.768 (13):0.232 (13) for the tetrafluoroborate anion and 0.5:0.5 for dichloromethane. The bond lengths and angles of the two components of the disordered atoms were restrained to be equal and refined isotropically.

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, 1997); software used to prepare material for publication: *SHELXTL*.

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