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Bis[2-(4,6-diphenyl-2-pyridyl)pyridine-κ^2N,N]copper(I) perchlorate dichloromethane solvate

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Key indicators

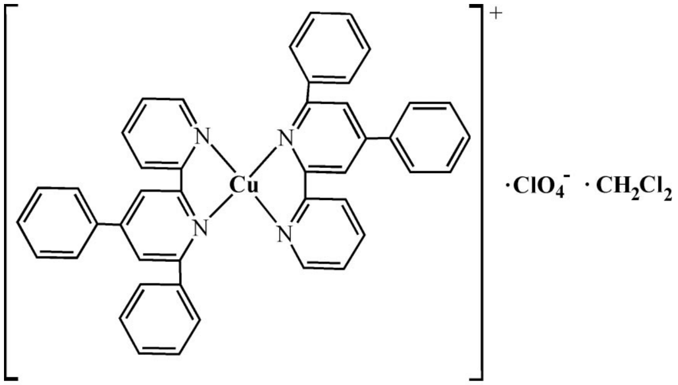
Single-crystal X-ray study
T = 130 K
Mean σ(C–C) = 0.005 Å
Disorder in solvent or counterion
R factor = 0.055
wR factor = 0.116
Data-to-parameter ratio = 16.0

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

The title compound, $[Cu(C_{22}H_{16}N_2)_2]ClO_4\cdot CH_2Cl_2$, was isolated from the reaction between $[Cu(PPh_3)_2(CH_3CN)_2]ClO_4$ and Pt(Ph-CNN)Cl [Ph-CNN is 2-(4,6-diphenyl-2-pyridyl)pyridine] in dichloromethane. The Cu atom adopts a distorted tetrahedral geometry.

Comment

Copper(I) bipyridine systems are of great interest because of their rich photoluminescent properties and the potential applications in electrochemistry (Williams *et al.*, 2002; Muller *et al.*, 1988). We report here the crystal structure of the copper(I) complex $[Cu(Ph\text{-}CNN)_2]ClO_4\cdot CH_2Cl_2$ [Ph-CNN is 2-(4,6-diphenyl-2-pyridyl)pyridine], which resulted from the reaction between $[Cu(PPh_3)_2(CH_3CN)_2]ClO_4$ and Pt(Ph-CNN)Cl in dichloromethane. A perspective view of the complex cation of (I) with the atomic numbering scheme is shown in Fig. 1.



(I)

As expected and often observed (Williams *et al.*, 2002; Muller *et al.*, 1988; Bardwell *et al.*, 1996), the complex cation is composed of a Cu^I ion coordinated by the N atoms of two Ph-CNN ligands, with Cu—N distances ranging between 2.001 (3) and 2.106 (2) Å; this range is similar to that previously determined for copper(I) bipyridine structures (Williams *et al.*, 2002; Bardwell *et al.*, 1995). The coordination geometry around the metal center is pseudo-tetrahedral, with the N—Cu—N angles varying between 80.45 (10) and 135.56 (10)°. The dihedral angle between the two bipyridine units is 66.0 (1)°. For each bipyridine unit, the two phenyl rings are tilted from the bipyridine ring plane by 45.2 (2) and 32.5 (2)°, and by 44.8 (2) and 38.4 (2)°. The perchlorate anion is disordered and this disorder was modeled by refining two discrete

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positions for each of the O atoms. No non-Coulombic interactions between the ClO_4^- anions and the cationic complex are observed.

Experimental

A mixture of $Cu(PPh_3)_2(CH_3CN)_2]ClO_4$ and Pt(Ph-CNN)Cl in a 1:2 molar ratio in dichloromethane was stirred under anaerobic conditions for 24 h. The reaction mixture was filtered to give a dark-red solution. Well shaped dark-red crystals suitable for X-ray diffraction measurements were grown by slow diffusion of light petroleum vapor into the filtrate at room temperature.

Crystal data

$[Cu(C_{22}H_{16}N_2)_2]ClO_4 \cdot CH_2Cl_2$
$M_r = 864.65$
Triclinic, $P\bar{1}$
$a = 11.035\ (4)$ Å
$b = 14.368\ (6)$ Å
$c = 14.637\ (6)$ Å
$\alpha = 114.257\ (2)^\circ$
$\beta = 101.688\ (2)^\circ$
$\gamma = 103.272\ (3)^\circ$
$V = 1940.6\ (13)$ Å^3
$Z = 2$
$D_x = 1.480$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3935 reflections
$\theta = 3.0$–27.5°
$\mu = 0.82$ mm^{-1}
$T = 130.2$ K
Prism, Red
$0.55 \times 0.20 \times 0.10$ mm

Data collection

Rigaku CCD diffractometer
Absorption correction: multi-scan (*SADABS*, Sheldrick, 1996)
$T_{min} = 0.825$, $T_{max} = 0.921$
15 105 measured reflections
8780 independent reflections
6621 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 27.5^\circ$
$h = -14 \rightarrow 7$
$k = -18 \rightarrow 18$
$l = -18 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.116$
$S = 1.07$
8780 reflections
550 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0307P)^2 + 2.7696P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.74$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}

H atoms were positioned geometrically (C—H = 0.97 or 0.93 Å), assigned isotropic displacement parameters [$U_{iso}(H) = 1.2U_{eq}(C)$] and allowed to ride on their respective parent C atoms.

Data collection: *CrystalClear* (Rigaku/MSC, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens 1994); software used to prepare material for publication: *SHELXL97*.

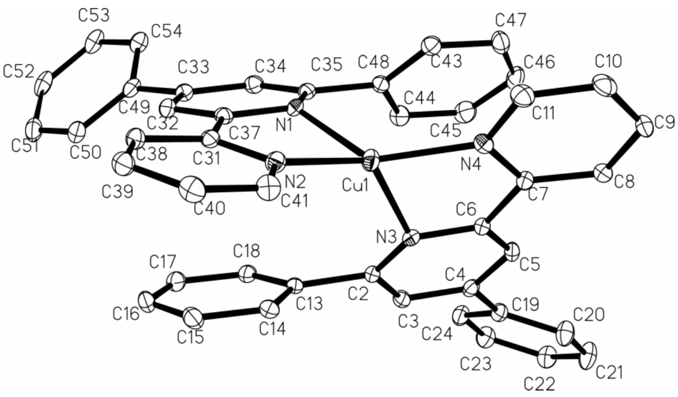

Figure 1
A view of the complex cation of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted.

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