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Bis(6,6′-dimethyl-2,2′-bipyridine)copper(I) perchlorate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
Disorder in solvent or counterion
R factor = 0.049
wR factor = 0.151
Data-to-parameter ratio = 14.3

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

In the title compound, $[Cu(C_{12}H_{12}N_2)_2]ClO_4$, the Cu^I atom is chelated by two heterocyclic ligands in a tetrahedral coordination geometry. The compound exists as cations and anions with only Coulombic interactions.

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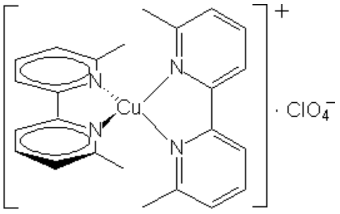
Comment

2,2'-Bipyridine forms a plethora of 2:1 adducts with Cu^I or Cu^{II} ions, in which the metal atom exhibits a coordination higher than four, as noted from a cursory search of the Cambridge Structural Database (November 2003 update; Allen, 2002). Methyl substituents in the 6,6′-positions effectively crowd the coordination polyhedron around the metal atom, and tetrahedral structures have been reported for the 4,4′,6,6′-tetramethyl-2,2′-bipyridine adducts of both copper(I) and copper(II) perchlorates (Burke, Henrick & McMillin, 1982) as well as that of copper(I) chloride (Dobson *et al.*, 1984).



(I)

The structure of tris(6,6′-dimethyl-2,2'-bipyridine)copper(I) tetrafluroborate has been described in detail (Burke, McMillin

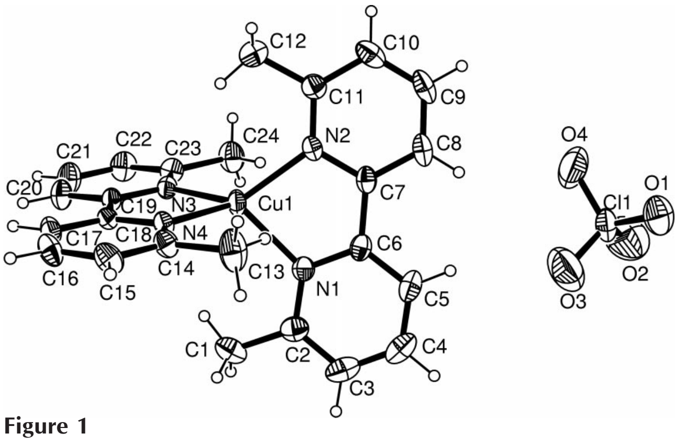


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), showing displacement ellipsoids at the 30% probability level. The site occupation factors of the perchlorate O atoms, O1–O4, are 50% each, and the other possible positions, O1′–O4′, have been omitted for clarity.

& Robinson, 1982); the title perchlorate, (I), is isostructural. The pair of compounds crystallize with similar cell dimensions. As shown in Fig. 1, the Cu atom is chelated by the two heterocyclic ligands in a tetrahedral coordination geometry. Selected bond lengths and angles are listed in Table 1.

Experimental

Compound (I) was obtained in an attempt to synthesize the dimethylbipyridine adduct of copper(I) phenylmalonate. To an aqueous methanol solution (30 ml; 1:1, *v*/*v*) of $Cu(ClO_4)_2 \cdot 6H_2O$ (0.37 g, 1.0 mmol) was added 6,6′-dimethyl-2,2′-bipyridine (0.18 g, 1.0 mmol) followed by disodium phenylmalonate (0.22 g, 1.0 mmol). The red solid that separated was collected and purified by recrystallization from acetonitrile to afford red bar-shaped crystals (yield *ca* 20%). Analysis calculated for $C_{24}H_{24}ClCuN_4O_4$: C 54.24, H 4.55, N 10.54%; found: C 54.15, H 4.53, N 10.48%.

Crystal data

$[Cu(C_{12}H_{12}N_2)_2]ClO_4$
$M_r = 531.46$
Monoclinic, $P2_1/c$
$a = 12.355$ (1) Å
$b = 21.912$ (2) Å
$c = 8.972$ (1) Å
$\beta = 95.58$ (1)°
$V = 2417.3$ (4) Å^3
$Z = 4$

$D_x = 1.460$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 844 reflections
$\theta = 1.7$–26.3°
$\mu = 1.05$ mm^{-1}
$T = 293$ (2) K
Bar, red
0.20 × 0.18 × 0.18 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min} = 0.817$, $T_{\rm max} = 0.833$
13 742 measured reflections

4892 independent reflections
3155 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.034$
$\theta_{\rm max} = 26.3°$
$h = -15 \rightarrow 15$
$k = -27 \rightarrow 26$
$l = -6 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.151$
$S = 1.03$
4892 reflections
343 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0781P)^2 + 1.2121P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.47$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.39$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.054 (3)	Cu1—N3	2.029 (3)
Cu1—N2	2.033 (3)	Cu1—N4	2.055 (3)
N1—Cu1—N2	81.6 (1)	N2—Cu1—N3	126.5 (1)
N1—Cu1—N3	127.8 (1)	N2—Cu1—N4	130.9 (1)
N1—Cu1—N4	115.3 (1)	N3—Cu1—N4	80.9 (1)
N1—C6—C7—N2	12.1 (5)	N4—C18—C19—N3	−2.8 (5)

The perchlorate O atoms show positional disorder, and they were refined as two groups sharing the same Cl atom. As the occupancy could not be satisfactorily refined, the eight O atoms were each given site occupancy of 0.5. The Cl—O and O···O distances were restrained with approximate equality. The displacement parameters of the disordered O atoms were also restrained weakly to be approximately isotropic. The aromatic [C—H = 0.93 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$] and methyl H atoms [C—H = 0.96 Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$] were included in the refinement in the riding-model approximation.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; method used to solve structure: atomic coordinates taken from the tetrafluoroborate structure; program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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