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Dichloro[3,3′-bis(ethoxycarbonyl)-2,2′-bipyridyl-κ^2N,N']copper(II)

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In the title compound, [$CuCl_2(C_{16}H_{16}N_2O_4)$], which crystallizes in the monoclinic space group *C*2/*c*, molecules are located on twofold rotation axes passing through the Cu centers and bisecting the bipyridyl ligands. They are interconnected by weak C—H···O and C—H···Cl interactions to form a two-dimensional network which stacks along the *c* axis.

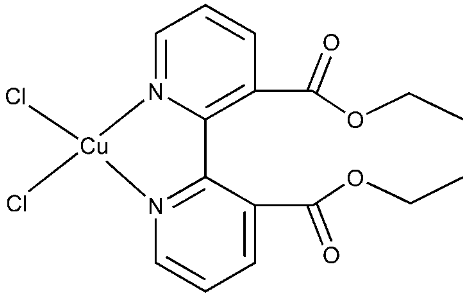
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.068
wR factor = 0.138
Data-to-parameter ratio = 13.2

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

Comment

Binicotinic acid, being a photoactive and multidentate ligand, has attracted much attention recently (Perkovic, 2000; Wu *et al.*, 2004). Moreover, the interesting emission properties of a platinum(II) complex with 3,3′-bis(methoxycarbonyl)-2,2′-bipyridyl has been reported by Miskowski *et al.* (1993). However, coordination compounds involving 3,3′-bis(ethoxycarbonyl)-2,2′-bipyridyl (DCEB) have not been exploited yet. We report here the first metal–DCEB coordination complex, [$CuCl_2$(DCEB)], (I), prepared from the reaction of $CuCl_2\cdot2H_2O$ and DCEB in CH_3CN.



(I)

X-ray diffraction analysis shows that (I) crystallizes in monoclinic space group *C*2/*c*. The local coordination geometry around each Cu^{II} center can be described as a severely distorted square (Fig. 1) in which each Cu^{II} center is coordinated by two N atoms from the 2,2′-pyridyl moiety of DCEB and two terminal chloride anions. The main deviation from the plane formed by atoms N1, Cl1, Cl1^{i}, N1^{i} (symmetry code as in Table 1) and Cu1 originates from its *trans* angles [146.67 (15)° for N1—Cu1—Cl1^{i} and N1^{i}—Cu1—Cl1], notably less than 180°, which leads to a coordination geometry close to that of a compressed tetrahedron. The dihedral angle between the two pyridine rings in (I) is 31.2 (5)°. The molecules are linked by weak C—H···O and C—H···Cl interactions to form a two-dimensional network which stacks along the *c* axis in the crystal (Fig. 2).

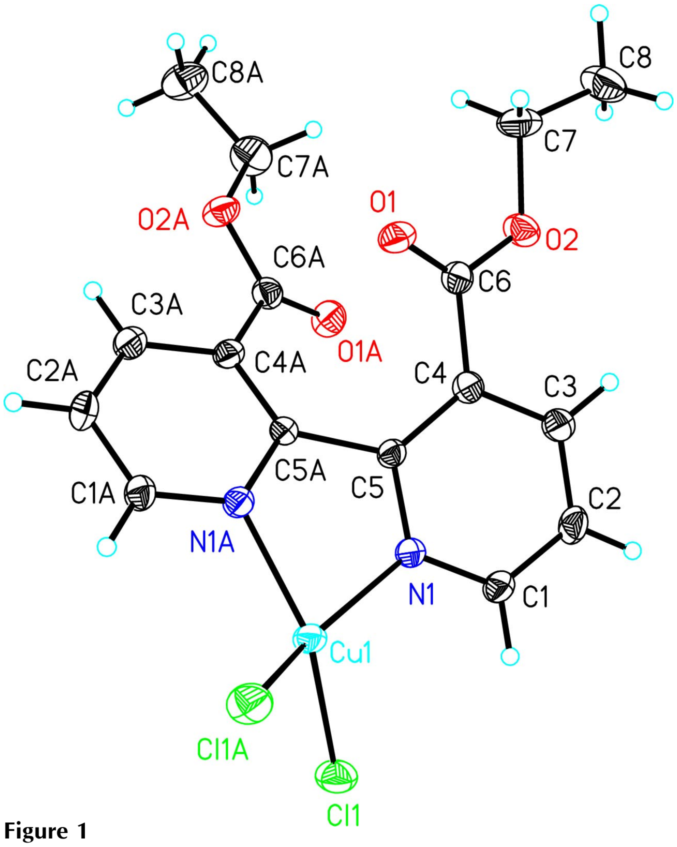


Figure 1
Perspective view of (I) with the atom-numbering scheme. Displacement ellipsoids are shown at the 30% probability level. The suffix A corresponds to symmetry code (i) in Table 1.

Experimental

The organic ligand DCEB was prepared by substitution of methanol with ethanol in the literature method of Dholakia *et al.* (1985). A mixture of DCEB (30 mg, 0.1 mmol), $CuCl_2.2H_2O$ (17 mg, 0.1 mmol) and CH_3CN (5 ml) was vigorously stirred for about 1 h to give a green solution. Slow evaporation of the resultant solution for two weeks produced green plate-like crystals suitable for X-ray diffraction.

Crystal data

$[CuCl_2(C_{16}H_{16}N_2O_4)]$
$M_r = 434.75$
Monoclinic, $C2/c$
$a = 11.3605$ (16) Å
$b = 11.2772$ (15) Å
$c = 13.5039$ (19) Å
$\beta = 91.269$ (3)°
$V = 1729.6$ (4) Å^3
$Z = 4$
$D_x = 1.670$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2620 reflections
$\theta = 2.6$–25.1°
$\mu = 1.60$ mm^{-1}
$T = 293$ (2) K
Plate, green
0.24 × 0.18 × 0.06 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.673$, $T_{max} = 0.909$
2620 measured reflections
1523 independent reflections
1238 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 25.1°$
$h = -10 \rightarrow 13$
$k = -13 \rightarrow 11$
$l = -13 \rightarrow 16$

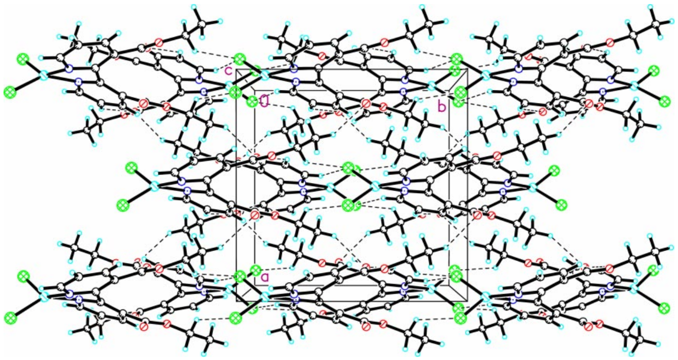


Figure 2
Packing diagram of (I), viewed along the *c* axis. Hydrogen-bond interactions are indicated by dashed lines.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.138$
$S = 1.23$
1523 reflections
115 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 18.8764P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.48$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.009 (5)	Cu1—Cl1	2.2082 (18)
N1^{i}—Cu1—N1	80.3 (3)	N1—Cu1—Cl1	97.01 (15)
N1^{i}—Cu1—Cl1	146.67 (15)	Cl1—Cu1—Cl1^{i}	102.45 (10)

Symmetry code: (i) $-x, y, \frac{3}{2} - z$.

H-atoms were positioned geometrically (C—H = 0.95–0.99 Å) and allowed to ride on their respective parent atoms, with $U_{iso}(H) = 1.2$ or 1.5 times $U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT* and *SHELXTL* (Sheldrick, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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