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Poly[(2,2′-bipyridine)copper(II)-μ_4-oxalato]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.015 Å
R factor = 0.051
wR factor = 0.108
Data-to-parameter ratio = 9.0

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

The crystal structure of the title compound, $[Cu(C_2O_4)(C_{10}H_8N_2)]_n$, is reported. The Cu^{II} atom is six-coordinated with distorted octahedral geometry and the bipyridine ligand acts as a chelating ligand. The oxalate anion bridges the metal ions forming infinite chains.

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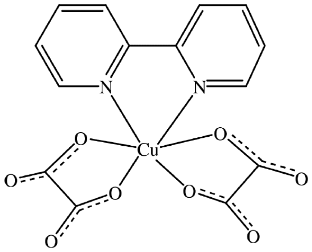
Comment

Oxalate-bridged polymeric compounds have attracted much attention due to their interesting magnetic properties (Decurtins *et al.*, 1994, and references therein). By reacting $CuCl_2$, 2,2′-bipyridine (2,2′-bipy) and tetrahydroxy-1,4-benzoquinone, the title complex, $[Cu(C_2O_4)(2,2'\text{-bipy})]_n$, was obtained, with oxalate anions as bridging ligands. So far, there have been only a few such compounds reported, *viz*. $[Cu(C_2O_4)(2,2'\text{-bipy})]\cdot 2H_2O$ (Fitzgerald *et al.*, 1982), $[Mn(C_2O_4)(2,2'\text{-bipy})]_n$ (Deguenon *et al.*, 1990) and $[Fe(C_2O_4)(2,2'\text{-bipy})]_n$ (Fun *et al.*, 1999).



(I)

The crystal structure of the title compound, which is isostructural with the Fe^{II} compound, consists of neutral $[Cu(C_2O_4)(2,2'\text{-bipy})]$ units, with the Cu atoms linked by C_2O_4 ligands to form infinite zigzag chains along the a axis. The Cu atom has a distorted octahedral coordination consisting of two N atoms from the chelating 2,2′-bipy ligand, two O atoms of the oxalate ligands in equatorial positions, and two O atoms of the oxalate ligands in axial positions. The largest deviation from the plane defined by Cu, N1, N2, O2 and O3^{i} is −0.089 Å at atom N1 [symmetry code: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, z$]. The Cu—N bond lengths [1.991 (7) and 2.018 (7) Å] and the N—Cu—N bite angle [80.4 (3)°] are comparable to the corresponding values in $[Cu_2(bipy)_2(H_20)_2(C_2O_4)]X_2\cdot[Cu(bipy)(C_2O_4)]$ (X = NO_3^-, BF_4 or ClO_4) [1.992 (2), 1.987 (2) Å and 82.92°; Gleizes *et al.*, 1992]. The Cu—O distances [1.972 (6)–2.369 (7) Å] and the O—Cu—O bite angles [90.6 (2) and 85.3 (3)°] are in agreement with those in $[Cu_2(bipy)_2(C_2O_4)(H_20)_2][Cu(bipy)(C_2O_4)](NO_3)_2$ [1.971 (1)–2.247 (1) Å and 84.64 (3)°; Shi *et al.*, 1997]; the bite angles are also close to those in $[Mn(C_2O_4)(2,2'\text{-bipy})]_n$ (Deguenon *et al.*, 1990) and

$[Fe(C_2O_4)(2,2'\text{-bipy})]_n$ (Fun *et al.*, 1999). The dihedral angle between the planar pyridyl rings is 2.01°. The shortest Cu···Cu distances within the chain is 5.507 Å. Neighbouring chains are connected to each other by van der Waals interactions, with the bipyridyl ligands stacked between the chains. The shortest Cu···Cu distance between adjacent chains is 7.793 Å.

Experimental

A solution of $CuCl_2\cdot6H_2O$ (0.085 g, 0.5 mmol) and tetrahydroxy-1,4-benzoquinone (0.10 g, 0.5 mmol) in methanol solution (20 ml) was stirred for 30 min at room temperature, then 2,2′-bipyridine (0.5 mmol) was added and the mixture was stirred for 1 h to give a green solution; this was filtered. Deep-green crystals were obtained by keeping the solution exposed to air for about a week. A green single-crystal was selected for X-ray diffraction.

Crystal data

$[Cu(C_2O_4)(C_{10}H_8N_2)]$
$M_r = 307.74$
Orthorhombic, $Pna2_1$
$a = 8.0762\ (11)$ Å
$b = 9.9366\ (13)$ Å
$c = 14.1558\ (19)$ Å
$V = 1136.0\ (3)$ Å^3
$Z = 4$
$D_x = 1.799$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 172 reflections
$\theta = 2.5$–$25.1°$
$\mu = 1.93$ mm^{-1}
$T = 293\ (2)$ K
Plate, green
0.35 × 0.28 × 0.21 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.408$, $T_{\max} = 0.458$
3348 measured reflections

1545 independent reflections
1084 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.060$
$\theta_{\max} = 25.1°$
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 6$
$l = -16 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.109$
$S = 1.05$
1545 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 0.3497P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.41$ e Å^{-3}
$\Delta\rho_{\min} = -0.46$ e Å^{-3}
Absolute structure: Flack (1983), 100 Friedel pairs treated independently
Flack parameter = 0.35 (4)

Table 1
Selected geometric parameters (Å, °).

Cu1—O2	1.972 (6)	Cu1—N2	2.018 (7)
Cu1—O3$^{\rm i}$	1.973 (6)	Cu1—O4	2.327 (6)
Cu1—N1	1.991 (7)	Cu1—O1$^{\rm i}$	2.369 (7)
O2—Cu1—O3$^{\rm i}$	90.6 (2)	N2—Cu1—O4	99.7 (2)
O2—Cu1—N1	94.5 (3)	O2—Cu1—O1$^{\rm i}$	85.3 (3)
O3$^{\rm i}$—Cu1—N2	94.9 (3)	O3$^{\rm i}$—Cu1—O1$^{\rm i}$	76.5 (2)
N1—Cu1—N2	80.4 (3)	N1—Cu1—O1$^{\rm i}$	98.2 (3)
O2—Cu1—O4	77.6 (2)	N2—Cu1—O1$^{\rm i}$	99.1 (3)
O3$^{\rm i}$—Cu1—O4	84.3 (2)		

Symmetry code: (i) $x - \frac{1}{2}, \frac{1}{2} - y, z$.

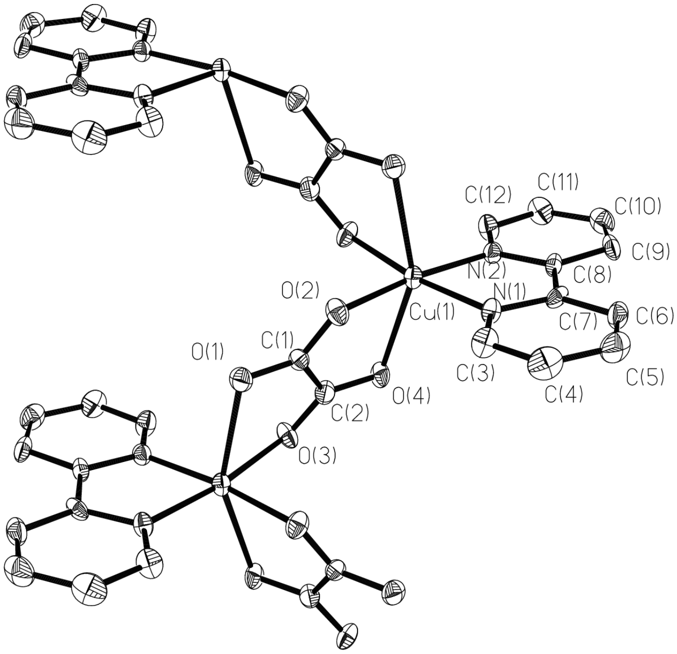


Figure 1
Part of the polymer chain of (I), showing 50% probability displacement ellipsoids and the labelling of the asymmetric unit.

H-atom positions were generated geometrically and the H atoms were allowed to ride on their respective parent C atoms.

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

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