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Key indicators

Single-crystal X-ray study
 T = 298 K
 Mean $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$
 R factor = 0.039
 wR factor = 0.103
 Data-to-parameter ratio = 12.9

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

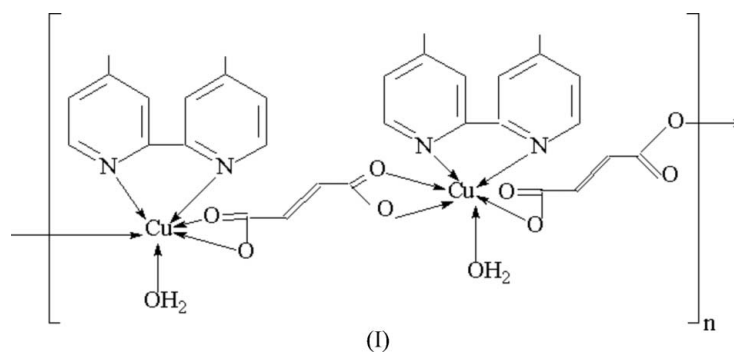
catena-Poly[[aqua(4,4'-dimethyl-2,2'-bipyridine)-copper(II)]- μ -fumarato- $\kappa^2\text{O},\text{O}'$: $\kappa^2\text{O}'',\text{O}'''$]-[aqua-(4,4'-dimethyl-2,2'-bipyridine)copper(II)]- μ -fumarato- $\kappa\text{O}:\kappa\text{O}'$]

The title compound, $[\text{Cu}(\text{C}_4\text{H}_2\text{O}_4)(\text{C}_{12}\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})]_n$, has a neutral polymeric chain structure in which fumarate ligands link the Cu atoms; the chains are then linked together by hydrogen bonds. The unique Cu^{II} ion exhibits a distorted octahedral coordination geometry defined by three O atoms of two different centrosymmetric fumarate ligands, two N atoms from the chelating dmbpy ligand (dmbpy is 4,4'-dimethyl-2,2'-bipyridine) and one water molecule. The fumarate ligands show two types of coordination modes, viz. bis-bidentate-chelating and bis-mono-O-carboxylate bridging.

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Comment

Metal complexes of carboxylates, especially polycarboxylates combined with chelating N,N' -donor ligands, are of immense interest in the construction of polymeric coordination architectures, owing to the fact that these polymers have a wide range of structural diversities and potential applications as porous materials and magnetic materials (Ye *et al.*, 2005). Some complexes in which the fumarate group acts as a bifunctional ligand, with 2,2'-bipyridyl and related auxiliary ligands, linking metal ions to construct polymeric frameworks have been synthesized and structurally investigated (Zheng *et al.*, 2004; Dalai *et al.*, 2002; Devereux *et al.*, 2000; Li *et al.*, 2002; Ma *et al.*, 2003; Wang *et al.*, 2000, 2002; Sun *et al.*, 2005). The structure of a new complex of this type, viz. the title compound, (I), is presented here.



The structure of (I) consists of polymeric chains running parallel to the *c* axis, in which the monomer is the unit $[\text{Cu}(\text{fumarato})_{2/2}(\text{dmbpy})(\text{H}_2\text{O})]$ (dmbpy is 4,4'-dimethyl-2,2'-bipyridine). In the chain, the Cu atoms are octahedrally coordinated by both N atoms of the bidentate chelating dmbpy ligand, one water molecule, and three O atoms of two different bridging fumarate ligands (Fig. 1). The water molecule and one of the fumarate O atoms (O4) are at the axial positions, with markedly longer Cu—O distances due to the

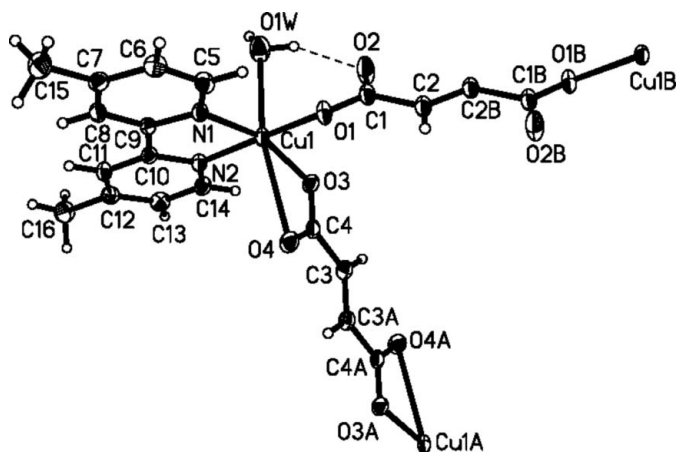


Figure 1

Part of the polymeric structure of (I), showing the Cu coordination environment. Displacement ellipsoids are drawn at the 30% probability level. Dashed lines indicate hydrogen bonds. [Symmetry codes: (A) $-x - 1, -y, -z + 1$; (B) $-x, -y, -z + 2$]

Jahn–Teller effect, so the coordination octahedron of the Cu atom is distorted. The Cu atom is displaced by 0.184 (1) Å from the equatorial plane towards the axial water molecule. The dihedral angle between the dmbpy ligand and the equatorial plane is 10.5 (1)°. The centrosymmetric fumarate ligands link the Cu atoms, one with bidentate and the other with monodentate coordination modes to form the neutral chains (Fig. 2). The carboxylate groups of the bridging fumarate ligands form O–H···O hydrogen bonds to water molecules (Table 2).

Experimental

A mixture of $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$ (120.5 mg, 0.5 mmol), fumaric acid (116 mg, 1 mmol), NaOH (80 mg, 2 mmol), dmbpy (184 mg, 1 mmol) and water (18 ml) was sealed in a 25 ml Teflon-lined stainless steel reactor and heated to 423 K for 72 h. The reactor was cooled to room temperature over a period of 24 h. Blue prismatic crystals suitable for X-ray diffraction analysis were obtained with a yield of 37%. Analysis calculated (%) for $\text{C}_{16}\text{H}_{16}\text{CuN}_2\text{O}_5$: C 50.59, H 4.25, N 7.37%; found (%): C 50.31, H 4.18, N 7.45%.

Crystal data

$[\text{Cu}(\text{C}_4\text{H}_2\text{O}_4)(\text{C}_{12}\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})]$	$Z = 2$
$M_r = 379.85$	$D_x = 1.572 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.337$ (3) Å	Cell parameters from 1020 reflections
$b = 10.767$ (5) Å	$\theta = 2.6\text{--}23.8^\circ$
$c = 10.967$ (5) Å	$\mu = 1.39 \text{ mm}^{-1}$
$\alpha = 93.602$ (7)°	$T = 298$ (2) K
$\beta = 104.926$ (7)°	Prism, blue
$\gamma = 104.640$ (7)°	$0.26 \times 0.22 \times 0.19 \text{ mm}$
$V = 802.3$ (6) Å ³	

Data collection

Bruker SMART CCD area-detector diffractometer	2597 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.017$
Absorption correction: none	$\theta_{\text{max}} = 25.5^\circ$
4286 measured reflections	$h = -8 \rightarrow 8$
2901 independent reflections	$k = -12 \rightarrow 13$
	$l = -13 \rightarrow 13$

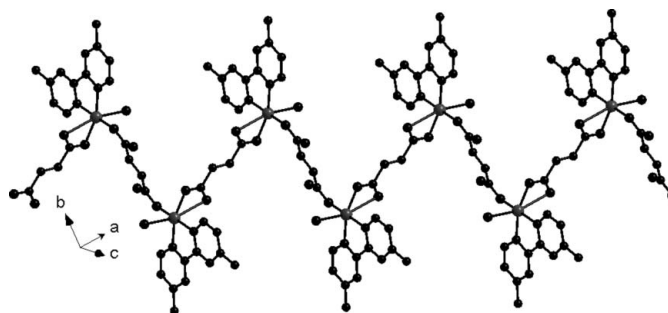


Figure 2

A view of the one-dimensional chain structure of (I). H atoms have been omitted for clarity.

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.039$
 $wR(F^2) = 0.103$
 $S = 1.03$
 2901 reflections
 225 parameters
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 0.3956P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.34 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.35 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cu1–O1	1.941 (2)	Cu1–N1	2.002 (2)
Cu1–O3	1.967 (2)	Cu1–O1W	2.400 (3)
Cu1–N2	1.993 (2)	Cu1–O4	2.684 (3)
O1–Cu1–O3	90.74 (9)	O3–Cu1–O1W	109.60 (10)
O1–Cu1–O4	87.34 (8)	N2–Cu1–O1W	93.40 (10)
O1–Cu1–N2	175.59 (9)	N1–Cu1–O1W	88.70 (10)
O3–Cu1–N2	91.48 (9)	O1W–Cu1–O4	163.87 (9)
O1–Cu1–N1	95.77 (9)	O3–Cu1–O4	54.68 (8)
O3–Cu1–N1	160.67 (9)	O4–Cu1–N1	107.37 (10)
N2–Cu1–N1	80.93 (9)	O4–Cu1–N2	90.84 (8)
O1–Cu1–O1W	89.45 (10)		

Table 2

Hydrogen-bond geometry (Å, °).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
O1W–HW1A···O4	0.84 (4)	2.04 (4)	2.869 (4)	166 (4)
O1W–HW1B···O2	0.84 (4)	1.94 (4)	2.708 (4)	152 (5)

Water H atoms were located in Fourier difference maps and refined isotropically, with an O–H distance restraint of 0.85 (1) Å. Other H atoms were placed in calculated positions, with C–H = 0.93 or 0.97 Å and refined with a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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, 1998); software used to prepare material for publication: SHELXTL.

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