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Poly[[[pyrazino[2,3-*f*][1,10]phenanthroline]-copper(II)]-μ_4-fumarato-μ_2-fumarato]

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In the title compound, $[Cu(C_4H_2O_4)(C_{14}H_8N_4)]$ or [Cu(fum)(Pyphen)], where fum is the fumarate dianion and Pyphen is pyrazino[2,3-*f*][1,10]phenanthroline, the Cu^{II} atom is five-coordinate in a distorted trigonal–bipyramidal geometry. The chelated Cu^{II} atoms are further bridged by the fum ligands to form a two-dimensional structure with (4,4)-grids.

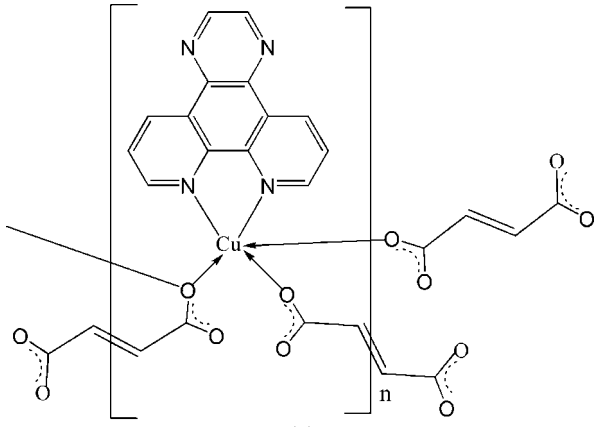
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.079
Data-to-parameter ratio = 14.2

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

Comment

Bridging aromatic polycarboxylate ligands such as 1,4-benzenedicarboxylate, 1,3-benzenedicarboxylate and 1,3,5-benzenetricarboxylate have been widely employed in the synthesis of coordination polymers (Eddaoudi *et al.*, 2001). Unsaturated organic acids such as fumaric acid are also interesting ligands for such polymers owing to their versatile coordination modes and varieties of structural conformations based on the terminal carboxylate groups. The fumarate ion as a flexible spacer has aroused enormous interest in recent years (Zhu *et al.*, 2006).



(I)

Metal dicarboxylato complexes with heteroaromatic N-donor chelating ligands have also been intensively studied (Chen & Liu, 2002), and the 1,10-phenanthroline (phen) ligand exemplifies such ligands. Pyrazino[2,3-*f*][1,10]phenanthroline (Pyphen) is a new phen derivative; however, the chemistry of supramolecular architectures based on Pyphen has received considerably less attention (Chen & Liu, 2002). We have selected fumaric acid (H_2fum) as a link and Pyphen as a secondary chelating ligand in the coordination polymer, [Cu(fum)(Pyphen)], (I), whose structure is reported here.

The Cu^{II} atom in (I) is five-coordinate and exhibits distorted trigonal–bipyramidal geometry (Fig. 1). Two carboxylate O atoms (O1 and O3) and one N atom (N1) from the Pyphen

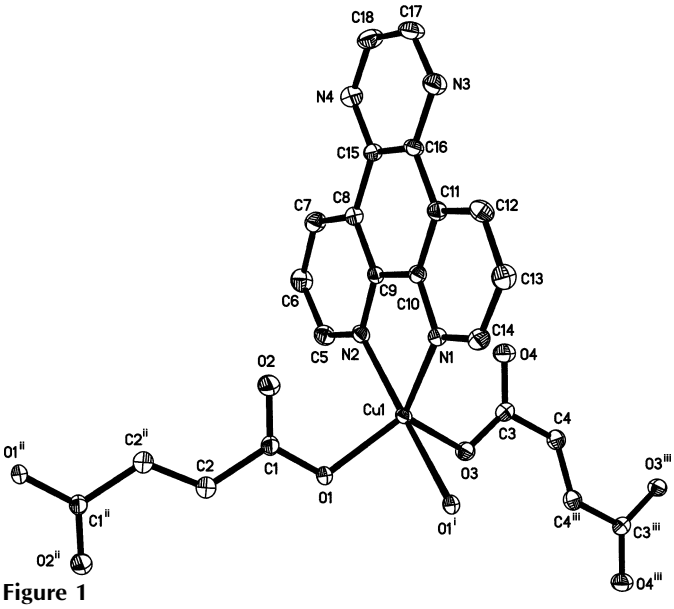


Figure 1
A segment of the polymeric structure of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $-x, -y, 1-z$; (ii) $-x, -1-y, 1-z$; (iii) $1-x, 1-y, 1-z$.]

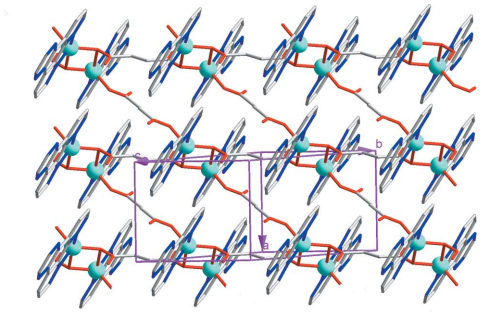


Figure 2
View of the two-dimensional layer structure of (I). H atoms have been omitted for clarity.

molecule form the equatorial plane, and atoms O1^{i} ($-x, -y, 1-z$) and N2 occupy the axial positions. The carboxylate groups of the fum ligands exhibit different coordination modes. One fum (fum1) ligand bridges four Cu^{II} atoms, whereas the other (fum2) connects two Cu^{II} atoms. The Cu^{II} ions are bridged by fum ligands to generate a two-dimensional structure with (4,4)-grids (Fig. 2). These layers are decorated with Pyphen ligands on both sides. Each corner of the (4,4)-grids is occupied by a binuclear Cu^{II} subunit.

Experimental

The Pyphen ligand was synthesized according to the method of Dickeson & Summers (1970). A methanol solution (6 ml) of Pyphen (0.5 mmol) was added slowly to an aqueous solution (15 ml) of $CuCl_2{\cdot}H_2O$ (0.5 mmol) and H_2fum (1 mmol) with stirring. The resulting solution was filtered and the filtrate was allowed to stand in air at room temperature for several days, yielding blue crystals of (I) (31% yield based on Cu).

Crystal data

$[Cu(C_4H_2O_4)(C_{14}H_8N_4)]$
$M_r = 409.84$
Triclinic, $P\overline{1}$
$a = 6.8545$ (14) Å
$b = 8.2037$ (16) Å
$c = 14.324$ (3) Å
$\alpha = 105.15$ (3)°
$\beta = 98.85$ (3)°
$\gamma = 94.75$ (3)°
$V = 761.8$ (3) Å^3
$Z = 2$
$D_x = 1.787$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.47$ mm^{-1}
$T = 292$ (2) K
Block, blue
0.33 × 0.31 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.604$, $T_{max} = 0.720$
7526 measured reflections
3467 independent reflections
2886 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.080$
$S = 1.06$
3467 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0299P)^2 + 0.4174P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.069 (2)	Cu1—O3	1.9546 (19)
Cu1—N2	2.116 (2)	Cu1—O1^{iii}	2.4085 (18)
Cu1—O1	1.9756 (17)		
O1—Cu1—O3	113.12 (8)	O3—Cu1—N2	104.66 (8)
O1—Cu1—N1	126.08 (8)	O3—Cu1—O1^{iii}	84.94 (7)
O1—Cu1—N2	102.27 (7)	N1—Cu1—N2	79.97 (8)
O1—Cu1—O1^{iii}	77.66 (7)	N1—Cu1—O1^{iii}	91.38 (7)
O3—Cu1—N1	118.28 (8)	N2—Cu1—O1^{iii}	169.30 (7)

Symmetry code: (iii) $-x+1, -y+1, -z+1$.

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and U_{iso}(H) set to 1.2U_{eq}(C).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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