Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Poly[[[(2,2′-bipyridine)copper(II)]-hemi-μ_2-2-nitroterephthalato-hemi-μ_4-2-nitroterephthalato] monohydrate]

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Received 18 January 2005
Accepted 1 February 2005
Online 12 February 2005

The polymeric title compound, $\{[Cu(C_8H_3NO_6)(C_{10}H_8N_2)]\cdot H_2O\}_n$, has two disordered nitroterephthalate units located around centres of inversion; one functions in a μ_2-bridging mode and the other in a μ_4-bridging mode to surround the five-coordinated Cu atom in a square-pyramidal geometry. The crystal structure reveals a two-dimensional hydrogen-bonded network involving a water molecule of crystallization.

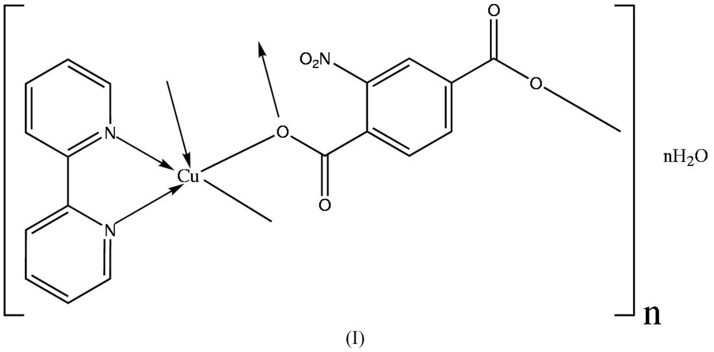
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.009 Å
Disorder in main residue
R factor = 0.052
wR factor = 0.108
Data-to-parameter ratio = 12.0

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

Comment

A previous study of copper 2-nitroterephthalate reported the inorganic–organic hybrid structure (Ma & Zhu, 2004); the compound exhibits a square-pyramidal coordination involving bridging dicarboxylate and hydroxyl groups, with the apical site of the pyramid occupied by a water molecule. The crystal structure is a three-dimensional network.



(I)

However, with the chelating 2,2′-bipyridine heterocycle, copper 2-nitroterephthalate adopts a only two-dimensional structure and does not include a coordinated water molecule, (I) (Fig. 1). The two symmetry-independent dianionic groups are each disordered over an inversion centre. One of the groups functions in the μ_2-bridging mode and the other in the μ_4-bridging mode to surround the five-coordinated Cu atom. The apical site of the square pyramid is occupied by the O atom of the μ_4-bridging dianion.

Experimental

A mixture of copper chloride dihydrate (0.035 g, 0.2 mmol), 2-nitroterephthalic acid (0.021 g, 0.1 mmol), 2,2′-bipyridine (0.032 g, 0.2 mmol), sodium hydroxide (0.008 g, 0.2 mmol) and water (8 ml) was sealed in a 25 ml stainless steel Teflon-lined bomb. The bomb was heated at 423 K for 3 d. After cooling, deep-blue block-shaped crystals of (I) were obtained.

Crystal data

$[Cu(C_8H_3NO_6)(C_{10}H_8N_2)]\cdot H_2O$
$M_r = 446.85$
Triclinic, $P\overline{1}$
$a = 9.537 (1)$ Å
$b = 9.950 (1)$ Å
$c = 11.363 (1)$ Å
$\alpha = 94.156 (2)^\circ$
$\beta = 107.839 (2)^\circ$
$\gamma = 113.535 (2)^\circ$
$V = 917.31 (16)$ Å^3
$Z = 2$
$D_x = 1.618$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 963 reflections
$\theta = 2.3$–20.4°
$\mu = 1.24$ mm^{-1}
$T = 295 (2)$ K
Block, blue
$0.23 \times 0.19 \times 0.17$ mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.764$, $T_{max} = 0.817$
5077 measured reflections
3534 independent reflections
2227 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 26.0^\circ$
$h = -11 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -14 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.108$
$S = 0.91$
3534 reflections
295 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0309P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O5	1.949 (3)	Cu1—N2	1.996 (4)
Cu1—O1	1.955 (3)	Cu1—O5^i	2.373 (3)
Cu1—N1	1.994 (4)		
O5—Cu1—O1	88.80 (12)	N1—Cu1—N2	80.84 (17)
O5—Cu1—N1	178.37 (15)	O5—Cu1—O5^i	77.27 (12)
O1—Cu1—N1	91.64 (15)	O1—Cu1—O5^i	89.05 (13)
O5—Cu1—N2	98.57 (14)	N1—Cu1—O5^i	104.30 (13)
O1—Cu1—N2	170.92 (15)	N2—Cu1—O5^i	97.70 (13)

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1W—H1W1$\cdots$O2	0.85 (6)	1.98 (6)	2.815 (6)	169 (6)
O1W—H1W2$\cdots$O6^{ii}	0.85 (5)	2.09 (4)	2.879 (7)	155 (8)

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

The aromatic H atoms were positioned geometrically, and were included in the refinement in the riding-model approximation [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. The water H atoms were located in a difference Fourier map and were refined with distance restraints of O—H = 0.85 (1) Å and H$\cdots$H = 1.39 (1) Å, and $U_{iso}(H) = 1.2U_{eq}(O)$. The two nitro groups are disordered with respect to H atoms; the C—N distances were restrained to 1.470 (5) Å, a tighter restraint being used to avoid too large a difference in distances. Additionally, the displacement parameters of the O atoms of the nitro groups were restrained to be nearly isotropic.

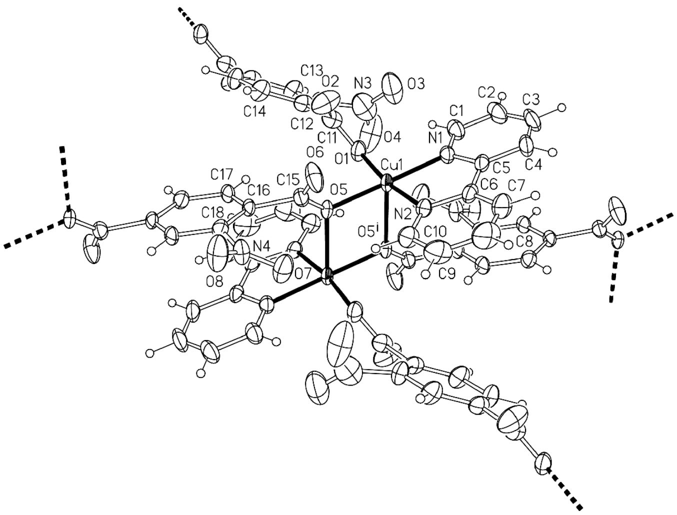


Figure 1
ORTEPII (Johnson, 1976) plot of a portion of the title compound. Displacement ellipsoids are drawn at the 50% probability level. The water molecules are not shown. [Symmetry code: (i) $1 - x, 1 - y, 1 - z$.]

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

We thank the Analytical and Measurement Fund of Zhejiang Province, the National Natural Science Foundation of China (grant No. 50073019) and the University of Malaya for supporting this study.

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