Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[[(2,2′-bipyridine)copper(II)]-μ-terephthalato] *N*,*N*-dimethylformamide solvate]

Xin-Hua Li and Hong-Ping Xiao*

Department of Chemistry and Materials Science, Wenzhou Normal College, Wenzhou 325027, People's Republic of China

Correspondence e-mail: hp_xiao@wznc.zj.cn

Received 17 May 2004
Accepted 25 May 2004
Online 5 June 2004

Key indicators

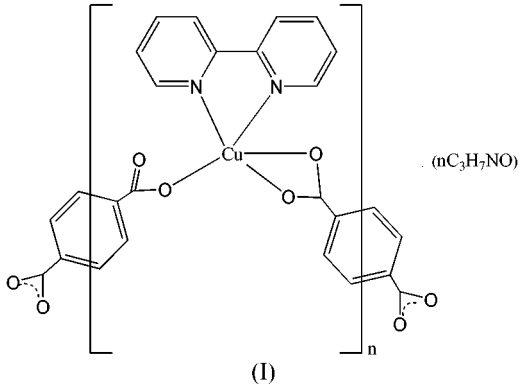
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.005 Å
R factor = 0.052
wR factor = 0.133
Data-to-parameter ratio = 13.3

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

In the title complex, $\{[Cu(C_8H_4O_4)(C_{10}H_8N_2)]\cdot C_3H_7NO\}_n$, each Cu atom is surrounded by three O atoms from two terephthalate dianions and two N atoms from a 2,2′-bipyridine molecule, forming a distorted square-pyramidal geometry. The terephthalate dianion functions as a bridge between two Cu atoms and forms a one-dimensional zigzag chain coordination polymer.

Comment

During the study of the structures of complexes in the Cu^{2+}/phen/H_2tp (phen is 1,10-phenanthroline and H_2tp is terephthalic acid) system (Cano *et al.*, 1997; Chen *et al.*, 2004; Sun *et al.*, 2000, 2001; Xiao *et al.*, 2004; Zhu *et al.*, 2004) and in the Cu^{2+}/2,2′-bipy/H_2ta (2,2′-bipy is 2,2′-bipyridine) system (Xiao & Zhu, 2003), we obtained a series of dinuclear complexes and one-dimensional zigzag chain coordination polymers. These complexes display a diversity of structures, and new complexes are constantly being produced through different reactions and even small changes, such as the use of different solvents, temperature, synthesis conditions or H-atom acceptors. All of these factors encouraged us to research these systems more deeply. Here, the title compound, [Cu(2,2′-bipy)(tp)]·(DMF), (I), represents an example.



(I)

In (I), the Cu atom is surrounded by three O atoms from two terephthalate dianions and two N atoms from a 2,2′-bipyridine molecule in a distorted square-pyramidal geometry (Fig. 1). The Cu1—N1 and Cu1—N2 bonds lengths are 1.996 (3) and 2.007 (3) Å, respectively. The apical position is occupied by atom O1, the corresponding axial Cu1—O1 [2.401 (3) Å] bond length being longer than the two basal [Cu1—O3^{i} = 1.930 (2) Å and Cu1—O2 = 1.992 (2) Å; symmetry code: (i) $x-\frac{1}{2}, y, \frac{1}{2}-z$] bonds lengths.

The terephthalate dianion functions as a bridge between two Cu atoms in a tridentate coordination mode. The 2,2′-

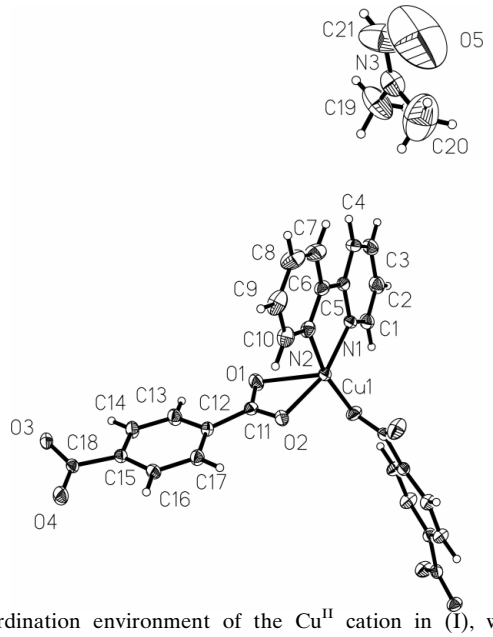


Figure 1
The coordination environment of the Cu^{II} cation in (I), with atom numbering for the asymmetric unit, showing displacement ellipsoids at the 50% probability level.

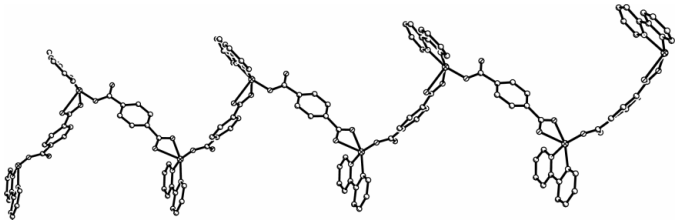


Figure 2
A view of the one-dimensional zigzag chain structure in (I); the DMF solvent molecules and H atoms have been omitted for clarity.

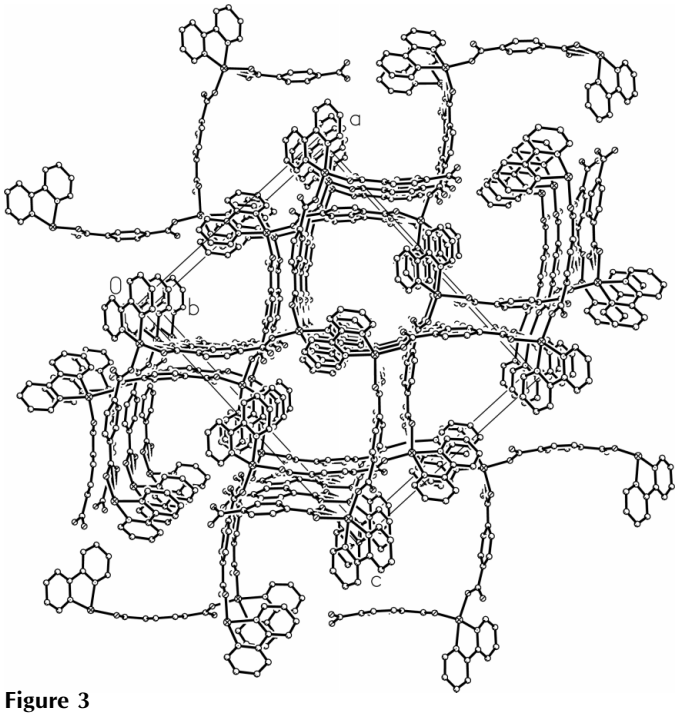


Figure 3
A view, down the *b* axis, of the packing; the DMF solvent molecules and H atoms have been omitted for clarity.

bipyridine group acts as a chelating ligand. A one-dimensional zigzag chain is formed by the Cu^{II} cations, the μ_2-bridging terephthalate dianions and the chelating 2,2′-bipyridine ligands (Fig. 2); this configuration is similar to that reported for [Cu(2,2′-bipy)(tp)(H_2O)](2H_2O)(DMF) (Xiao & Zhu, 2003). Moreover, there are π–π interactions involving the 2,2′-bipyridine ligands belonging to adjacent zigzag chains, with a distance of about 3.45 Å. Adjacent zigzag chains interweave with each other to generate a two-dimensional network structure with cavities (Fig. 3). The DMF solvent molecules fill the cavities.

Experimental

A solution (10 ml) of dimethylformamide containing $Cu_2Cl_2{\cdot}2H_2O$ (0.3 mmol) was added dropwise to a solution (10 ml) of dimethylformamide containing 2,2′-bipyridine (0.3 mmol), terephthalic acid (0.3 mmol) and 1,1′-carbonyldiimidazole (0.3 mmol) at room temperature. The reaction mixture was filtered and the filtrate was left to stand for about two weeks until blue single crystals were obtained.

Crystal data

$[Cu(C_8H_4O_4)(C_{10}H_8N_2)]{\cdot}C_3H_7NO$
M_r = 456.94
Orthorhombic, *Pbca*
a = 16.6884 (7) Å
b = 10.9585 (5) Å
c = 22.0082 (9) Å
V = 4024.9 (3) Å^3
Z = 8
D_x = 1.508 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3619 reflections
θ = 2.4–23.0°
μ = 1.12 mm^{-1}
T = 273 (2) K
Prism, blue
0.27 × 0.18 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.784, T_{max} = 0.863
19 899 measured reflections
3619 independent reflections
3139 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 25.2°
$h = -19 \rightarrow 14$
$k = -13 \rightarrow 12$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.133
S = 1.10
3619 reflections
273 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0642P)^2 + 5.3628P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O3^{i}	1.930 (2)	Cu1—N2	2.007 (3)
Cu1—O2	1.992 (2)	Cu1—O1	2.401 (3)
Cu1—N1	1.996 (3)		
O3^{i}—Cu1—O2	95.50 (11)	O2—Cu1—N1	162.16 (11)
O3^{i}—Cu1—N1	94.38 (11)	O3^{i}—Cu1—N2	166.37 (12)

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

H atoms attached to C atoms were included in the refinement in calculated positions in the riding-model approximation [C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for Csp^3].

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve

structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the Wenzhou S & T Project of China (grant No. S2003A008).

References

Bruker (2000). *SMART* (Version 5.618), *SAINT* (Version 6.02a), *SADABS* (Version 2.03) and *SHELXTL* (Version 5.03). Bruker AXS Inc., Madison, Wisconsin, USA.

Cano, J., Munno, G. D., Sanz, J. L., Ruiz, R., Fanus, J., Lloret, F., Julve, M. & Caneschi, A. (1997). *J. Chem. Soc. Dalton Trans.* pp. 1915–1923.

Chen, F., Li, X.-H., Xiao, H.-P. & Hu, M.-L. (2004). *Acta Cryst.* E**60**, m708–m710.

Sun, D.-F., Cao, R., Liang, Y.-C., Hong, M.-C., Su, W.-P. & Weng, J.-B. (2000). *Acta Cryst.* C**56**, e240–e241.

Sun, D.-F., Cao, R., Liang, Y.-C., Shi, Q., Su, W.-P. & Hong, M.-C. (2001). *J. Chem. Soc. Dalton Trans.* pp. 2335–2340.

Xiao, H.-P., Li, X.-H., Ye, M.-D. & Hu, M.-L. (2004). *Acta Cryst.* E**60**, m253–m254.

Xiao, H.-P. & Zhu, L.-G. (2003). *Chin. J. Inorg. Chem.* **19**, 1179–1183.

Zhu, L.-G., Xiao, H.-P. & Lu, J.-Y. (2004). *Inorg. Chem. Commun.* **7**, 94–96.