

**catena-Poly[[[μ -4,4'-bipyridine-bis[aquacopper(II)]]-
di- μ -2-nitroterephthalato]****Hong-Yin He,^a Long-Guan Zhu^{a*}
and Seik Weng Ng^b**^aDepartment of Chemistry, Zhejiang University, Hangzhou 310007, People's Republic of China, and ^bDepartment of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia

Correspondence e-mail: chezlg@zju.edu.cn

Key indicatorsSingle-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
Disorder in main residue
 R factor = 0.050
 wR factor = 0.137
Data-to-parameter ratio = 12.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title polymeric compound, $[\text{Cu}_2(\text{C}_8\text{H}_3\text{NO}_6)_2(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2]_n$, the unique Cu atom, the water molecule and the nitrogen heterocycle lie on mirror planes, and the disordered nitrophthalate dianion lies on a twofold axis. The Cu atom shows square-planar coordination as it is bonded to the O atoms of two carboxyl groups, to the N atom of a pyridyl ring and to a water molecule.

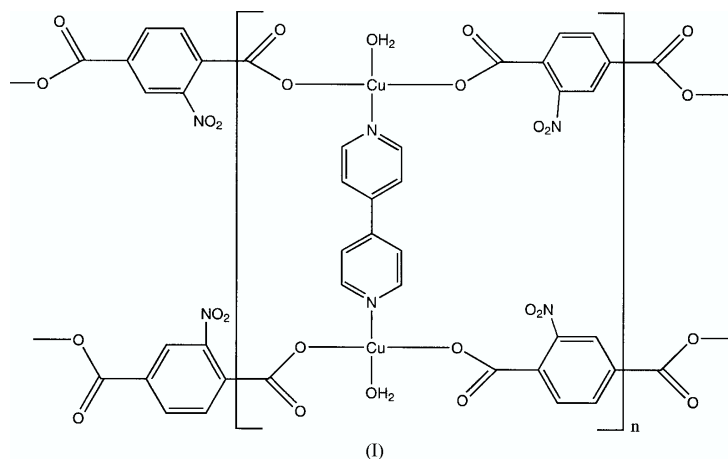
Received 21 January 2005

Accepted 22 February 2005

Online 26 February 2005

Comment

Although the terephthalate dianion has been used as the dicarboxylate counter-ion for the synthesis of transition metal carboxylates, and although the 4,4'-bipyridine nitrogen heterocycle has been used as a spacer ligand in a plethora of adducts with transition metal carboxylates, there is only one example of a system that exhibits both features, *i.e.* a rigid terephthalate dianion and a rigid spacer molecule (Tao *et al.*, 2000). This zinc complex has the dianion engaged in both μ_2 - and μ_4 -bridging modes. A similar reaction with a copper salt as the reagent yielded the title compound, (I) (Fig. 1); both the dianion and spacer units function in the expected μ_2 -bridging modes, but the metal atom shows only square-planar geometry. The bridging modes lead to the formation of a two-dimensional network architecture that is consolidated further by hydrogen bonds.



The unique Cu atom, the water molecule and the nitrogen heterocycle lie on mirror planes, and the disordered nitrophthalate dianion lies on a twofold axis.

Experimental

Copper nitrate dihydrate (0.074 g, 0.31 mmol), 2-nitrobenzene-1,4-dicarboxylic acid (0.066 g, 0.31 mmol), 4,4'-bipyridine (0.048 g,

0.31 mmol) and water (10 ml) were sealed in a 20 ml Teflon-lined stainless steel reactor. The reactor was heated to 413 K for 24 h. After it was cooled, block-shaped deep-blue crystals were obtained.

Crystal data

[Cu₂(C₈H₃NO₆)₂(C₁₀H₈N₂)(H₂O)₂] Mo K α radiation
M_r = 737.52 Cell parameters from 1365 reflections
 Orthorhombic, *Cmca* θ = 2.4–23.2°
a = 21.662 (2) Å μ = 1.67 mm⁻¹
b = 16.726 (2) Å *T* = 295 (2) K
c = 7.405 (1) Å Block, blue
V = 2683.0 (5) Å³ 0.29 × 0.15 × 0.12 mm
Z = 4
D_x = 1.826 Mg m⁻³

Data collection

Bruker SMART area-detector 1579 independent reflections
 diffractometer 980 reflections with *I* > 2 σ (*I*)
 φ and ω scans *R*_{int} = 0.082
 Absorption correction: multi-scan θ _{max} = 27.5°
 (SADABS; Bruker, 2001) *h* = -27 → 18
*T*_{min} = 0.656, *T*_{max} = 0.825 *k* = -21 → 21
 7488 measured reflections *l* = -9 → 9

Refinement

Refinement on *F*² H-atom parameters constrained
R [*F*² > 2 σ (*F*²)] = 0.050 *w* = 1/[$\sigma^2(F_o^2) + (0.0768P)^2$]
wR (*F*²) = 0.137 where *P* = (*F_o*² + 2*F_c*²)/3
S = 0.92 (Δ / σ)_{max} = 0.001
 1579 reflections $\Delta\rho$ _{max} = 0.64 e Å⁻³
 125 parameters $\Delta\rho$ _{min} = -0.49 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1–O1	1.939 (3)	Cu1–N1	1.993 (5)
Cu1–O1w	1.928 (5)		
O1–Cu1–O1 ⁱ	170.0 (2)	O1–Cu1–N1	93.1 (1)
O1–Cu1–O1w	86.8 (1)	O1w–Cu1–N1	178.9 (2)

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

The nitro group has only half-occupancy and it is disordered together with an H atom. The group was refined with a C–N distance restraint of 1.47 (1) Å and an N–O distance restraint of 1.21 (1) Å. Additionally, the displacements of its two O atoms were restrained to be approximately isotropic. The carbon-bound H atoms were positioned geometrically [C–H = 0.93 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C)] and were included in the refinement in the riding-model approximation. The unique H atom of the O1w water molecule was positioned to fit the electron density [O–H = 0.85 Å and *U*_{iso}(H) = 1.2*U*_{eq}(O)].

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); 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 Shanghai Institute of Organic Chemistry for the diffraction measurements, and the National Natural Science Foundation of China (grant No. 50073019) and the University of Malaya for supporting this study.

References

Bruker (2001). SADABS, SAINT and SMART. Bruker AXS Inc., Madison, Wisconsin, USA.

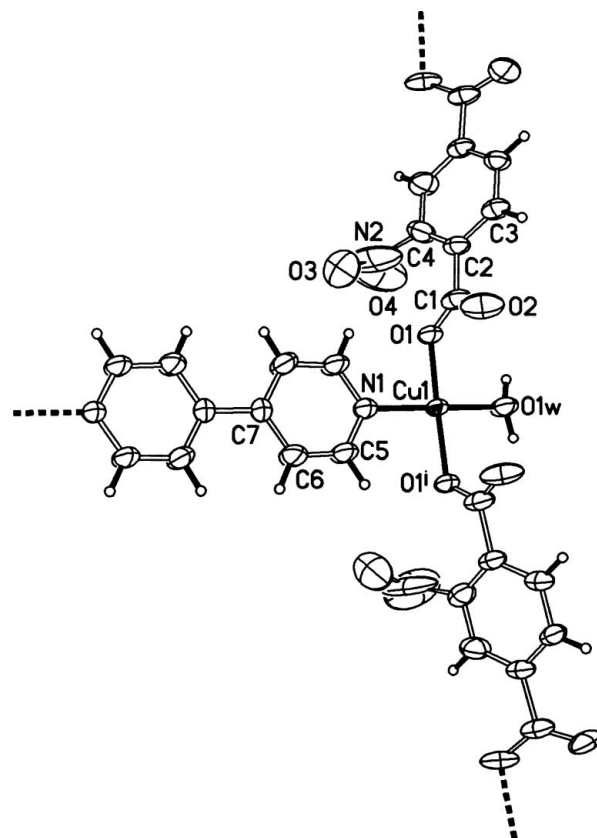


Figure 1

ORTEPII plot (Johnson, 1976) of a fragment of the polymeric structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. Dashed lines represent bonds to adjacent structural units. [Symmetry code: (i) 1 - *x*, *y*, *z*.]

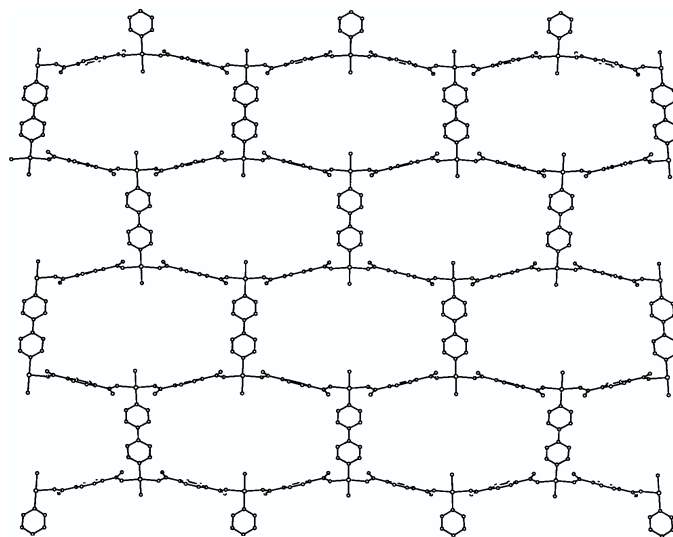


Figure 2

View of the two-dimensional network in (I). Nitro groups and H atoms have been omitted for clarity.

Johnson, C. K. (1976). ORTEPII. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.

Tao, J., Tong, M.-L. & Chen, X.-M. (2000). *J. Chem. Soc. Dalton Trans.* pp. 3669–3674.