

Guang-Bo Che,* Chun-Bo Liu,
Yun-Cheng Cui and Chuan-Bi LiDepartment of Chemistry, Jilin Normal University,
Siping 136000, People's Republic of ChinaCorrespondence e-mail:
guangbochejl@yahoo.com

Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.046
 wR factor = 0.123
Data-to-parameter ratio = 13.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Diaquatetrakis(μ -2-phenylquinoline-4-carboxylato- $\kappa^2\text{O}:\text{O}'$)dicopper(II)($\text{Cu}-\text{Cu}$)

The title complex, $[\text{Cu}_2(\text{C}_{16}\text{H}_{10}\text{NO}_2)_4(\text{H}_2\text{O})_2]$, has a centrosymmetric wheel-shaped dinuclear structure in which two symmetry-related Cu^{II} centers are bridged by four carboxylate groups of distinct 2-phenylquinoline-4-carboxylate (phqc) ligands, the $\text{Cu}-\text{Cu}$ separation being 2.6507 (12) Å. Each Cu^{II} center is five-coordinated by four O atoms of carboxylate groups in the basal plane and one O atom of a water molecule in the apical position. In addition, the dinuclear molecules are linked by intermolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds to form a one-dimensional supramolecular chain.

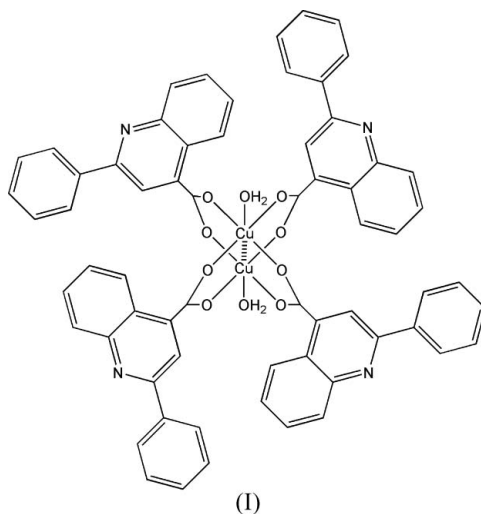
Received 17 October 2005

Accepted 25 October 2005

Online 31 October 2005

Comment

2-Phenylquinoline-4-carboxylic acid (Hphqc) is a potential multi-functional ligand containing carboxylate group and nitrogen coordination donors, and possesses rich coordination and structural chemistry. Its crystal structure has been reported by Blackburn *et al.* (1996). However, the investigation of its metal complexes, especially their crystal structure determinations, are rare (Qin *et al.*, 1999, 2002; Parish *et al.*, 2000). We report here the synthesis and crystal structure of a dinuclear copper complex $[\text{Cu}(\text{phqc})_2(\text{H}_2\text{O})_2]$, (I), with this ligand.



As shown in Fig. 1, complex (I) is a neutral molecule with a centrosymmetric wheel-shaped dinuclear structure, in which there are two crystallographically identical Cu^{II} centers bridged by four carboxylate groups of four distinct phqc ligands. Each Cu^{II} center is five-coordinated by four O atoms of carboxylate groups in the basal plane and one O atom of a water molecule in the apical position to give an almost ideal square-pyramidal coordination environment. The Cu^{II} ion

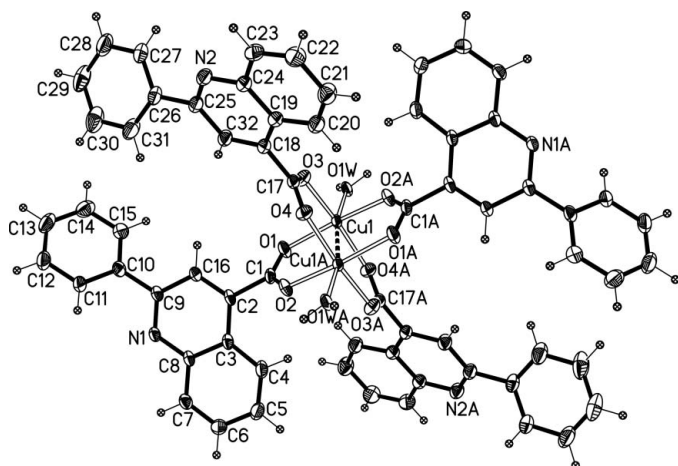


Figure 1
Structure of (I), showing displacement ellipsoids at the 30% probability level [symmetry code: (A) $1 - x, 1 - y, -z$].

deviates from the mean basal plane of the square pyramid toward the apical O1W atom by 0.211 (2) Å. The Cu—Cu distance (see Table 1) in the dinuclear unit is well below the summed van der Waals radii of two Cu atoms (2.8 Å). As listed in Table 1, the apical Cu—O distance [Cu1—O1W] is significantly longer than those in the basal plane [those four are almost equivalent, the average value being 1.969 (2) Å] as a result of the strong Jahn–Teller effect of Cu^{II}. The phqc ligands in (I) adopt a μ_2 -bridging coordination mode using two O atoms of carboxylate group with the N atom uncoordinated. The dihedral angles between the carboxylate planes and the quinoline groups are 58.7 (2)° for O1/C1/O2 and C2—C9/C16/N1, and 56.8 (2)° for O3/C17/O4 and C18—C25/C32/N2. It should be noted that a one-dimensional supramolecular chain structure is formed through intermolecular O—H...N hydrogen-bonding interactions between coordinated water molecules and uncoordinated nitrogen donors of quinoline (Table 2).

Experimental

Complex (I) was synthesized hydrothermally under autogenous pressure; a mixture of Hphqc, Cu(NO₃)₂·6H₂O and water in a molar ratio of 2:1:5000 was sealed in a Teflon-lined autoclave and heated to 433 K for 2 d. Blue crystals were obtained in ca 10% yield based on copper(II). IR (KBr pellet, cm⁻¹): 3642 (*m*), 3358 (*w*), 3057 (*w*), 1627 (*s*), 1592 (*s*), 1549 (*m*), 1509 (*w*), 1459 (*w*), 1433 (*s*), 1397 (*s*), 1325 (*m*), 1236 (*w*), 1159 (*w*), 1080 (*w*), 1027 (*m*), 896 (*m*), 766 (*s*), 693 (*s*), 651 (*m*), 569 (*w*), 548 (*w*), 523 (*w*), 466 (*m*).

Crystal data

[Cu₂(C₁₆H₁₀NO₂)₄(H₂O)₂]
 $M_r = 1156.11$
 Triclinic, $P\bar{1}$
 $a = 8.2800$ (17) Å
 $b = 10.668$ (2) Å
 $c = 15.501$ (3) Å
 $\alpha = 86.62$ (3)°
 $\beta = 85.99$ (3)°
 $\gamma = 70.92$ (3)°
 $V = 1289.9$ (4) Å³

$Z = 1$
 $D_x = 1.488$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 10366 reflections
 $\theta = 3.1$ – 27.5 °
 $\mu = 0.89$ mm⁻¹
 $T = 293$ (2) K
 Block, blue
 0.14 × 0.10 × 0.10 mm

Data collection

Rigaku R-Axis RAPID
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.885, T_{\max} = 0.916$
 10554 measured reflections

4730 independent reflections
 3963 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$
 $\theta_{\max} = 25.5$ °
 $h = -10 \rightarrow 10$
 $k = -12 \rightarrow 11$
 $l = -18 \rightarrow 18$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.123$
 $S = 1.06$
 4730 reflections
 361 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0735P)^2 + 0.2379P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.04$ e Å⁻³
 $\Delta\rho_{\min} = -0.47$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.962 (2)	Cu1—O4 ⁱ	1.973 (2)
Cu1—O2 ⁱ	1.976 (2)	Cu1—O1W	2.167 (2)
Cu1—O3	1.966 (2)	Cu1—Cu1 ⁱ	2.6507 (12)
O1—Cu1—O1W	99.22 (9)	O3—Cu1—O1W	99.58 (9)
O1—Cu1—O2 ⁱ	167.50 (9)	O3—Cu1—O2 ⁱ	88.61 (10)
O1—Cu1—O3	88.27 (10)	O3—Cu1—O4 ⁱ	167.74 (9)
O1—Cu1—O4 ⁱ	89.97 (10)	O4 ⁱ —Cu1—O1W	92.67 (9)
O2 ⁱ —Cu1—O1W	93.24 (8)	O4 ⁱ —Cu1—O2 ⁱ	90.51 (10)

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

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1W—H2...N1 ⁱⁱ	0.84	2.05	2.873 (3)	169

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

H atoms bonded to C atoms were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The H atoms of the water molecules were located in difference Fourier maps and their positions were held fixed in the least-squares refinement with isotropic displacement parameters set at $1.2U_{\text{eq}}(\text{O})$. The highest electron-density peak is located at (0.4425, 0.1216, 0.3355).

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *SHELXL97*.

The authors thank Jilin Normal University for supporting this work.

References

- Blackburn, A. C., Dobson, A. J. & Gerkin, R. E. (1996). *Acta Cryst.* **C52**, 409–411.
 Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
 Parish, R. V., Wright, J. P. & Pritchard, R. G. (2000). *J. Organomet. Chem.* **596**, 165–176.
 Qin, Z., Jenkins, H. A., Coles, S. J., Muir, K. W. & Puddephatt, R. J. (1999). *Can. J. Chem.* **77**, 155–157.

Qin, Z., Jennings, M. C., Puddephatt, R. J. & Muir, K. W. (2002). *Inorg. Chem.* **41**, 5174–5186.

Rigaku Corporation (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.

Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc., 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.

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