

**Hong-Song Li, Song-Lin Li\* and  
Jian-Feng Hou**Department of Chemistry, Tianjin University,  
Tianjin 300072, People's Republic of China

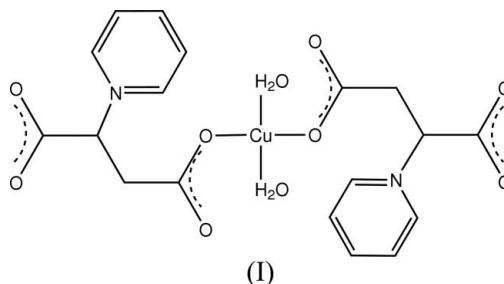
Correspondence e-mail: lihongsong@sohu.com

**Key indicators**Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.025  
 $wR$  factor = 0.070  
Data-to-parameter ratio = 14.2For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**Diaquabis[2-(1-pyridyl)butanedioato- $\kappa$ O]copper(II)**

The crystal structure of the title complex,  $[\text{Cu}(\text{C}_9\text{H}_8\text{NO}_4)_2(\text{H}_2\text{O})_2]$ , consists of discrete  $\text{Cu}^{\text{II}}$  complex molecules, which are linked to each other by classical  $\text{O}-\text{H}\cdots\text{O}$  and weak  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonding. The  $\text{Cu}^{\text{II}}$  ion is located on an inversion centre and coordinated by two water molecules and two carboxylate groups from two 2-(1-pyridyl)butanedioate ligands, with a square-planar geometry.

Received 5 April 2006  
Accepted 27 May 2006**Comment**

Polymeric metal complexes bridged by carboxylate anions have been reported. During the preparation of polymeric complexes using 2-(1-pyridyl)butanedioate as a bridging ligand, we obtained crystals of the title monomeric  $\text{Cu}^{\text{II}}$  complex, (I). In this report, we present the crystal structure of (I).



As shown in Fig. 1, the  $\text{Cu}^{\text{II}}$  ion is located on an inversion centre and is coordinated by two water molecules and two carboxylate groups from two 2-(1-pyridyl)butanedioate ligands, with a square-planar geometry (Table 1). The other carboxylate group of the 2-(1-pyridyl)butanedioate ligand is free from coordination but is hydrogen-bonded to the coordinated water molecule of a neighbouring complex.  $\text{O}-\text{H}\cdots\text{O}$  and weak  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonding occurs in the crystal structure of (I) (Table 2).

**Experimental**

2-(1-Pyridyl)butanedioic acid (*L*) was prepared according to the procedure of Kostyanovsky *et al.* (2003). An aqueous solution of NaL (0.217 g, 1 mmol) and  $\text{Cu}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$  (0.370 g, 1 mmol) was stirred for 6 min at 333 K and then left to stand at room temperature. Single crystals of (I) were obtained after 5 d.

*Crystal data*

$[\text{Cu}(\text{C}_9\text{H}_8\text{NO}_4)_2(\text{H}_2\text{O})_2]$   
 $M_r = 487.90$   
Monoclinic,  $P2_1/n$   
 $a = 5.109$  (1) Å  
 $b = 19.187$  (4) Å  
 $c = 10.290$  (2) Å  
 $\beta = 103.30$  (3)°  
 $V = 981.6$  (4) Å<sup>3</sup>

$Z = 2$   
 $D_x = 1.651$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
 $\mu = 1.17$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
Block, blue  
0.25 × 0.23 × 0.20 mm

Data collection

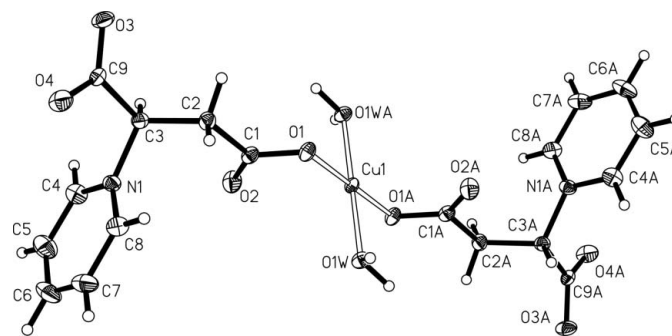
Bruker SMART 1000 CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.743$ ,  $T_{\max} = 0.790$

5019 measured reflections  
 2016 independent reflections  
 1739 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.020$   
 $\theta_{\text{max}} = 26.4^\circ$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.025$   
 $wR(F^2) = 0.070$   
 $S = 1.07$   
 2016 reflections  
 142 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 0.3152P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.31 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.26 \text{ e } \text{\AA}^{-3}$



**Figure 1**  
 The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms) [symmetry code: (A)  $-x, -y, 1 - z$ ].

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Cu1—O1	1.9468 (13)	Cu1—O1W	1.9442 (12)
O1W—Cu1—O1	89.03 (5)		

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1W—H1WA $\cdots$ O1 <sup>i</sup>	0.89	1.85	2.7309 (19)	172
O1W—H1WB $\cdots$ O3 <sup>ii</sup>	0.92	1.66	2.5812 (17)	175
C2—H2B $\cdots$ O2 <sup>iii</sup>	0.97	2.57	3.542 (3)	176
C3—H3A $\cdots$ O4 <sup>iv</sup>	0.98	2.56	3.470 (2)	154
C4—H4A $\cdots$ O4 <sup>iv</sup>	0.93	2.31	3.193 (3)	159
C7—H7A $\cdots$ O4 <sup>v</sup>	0.93	2.52	3.407 (3)	160
C8—H8A $\cdots$ O2 <sup>iii</sup>	0.93	2.39	3.320 (3)	174

Symmetry codes: (i)  $-x + 1, -y, -z + 1$ ; (ii)  $x, y, z + 1$ ; (iii)  $x + 1, y, z$ ; (iv)  $x - 1, y, z$ ; (v)  $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ .

Water H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ . Other H atoms were placed in calculated positions, with  $C-H = 0.93$  to  $0.98 \text{ \AA}$ , and refined in riding mode with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

References

Bruker (1997). SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Bruker (1998). SMART and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Kostyanovsky, R. G., Nikolaev, E. N., Kharybin, O. N., Kadorkina, G. K. & Kostyanovsky, V. R. (2003). Mendeleev Commun., 97–99.  
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.