Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Catena-poly[aqua(2,2′-bipyridine)copper(II)-μ-benzene-1,4-dioxyacetato]

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Received 5 April 2005
Accepted 12 April 2005
Online 16 April 2005

In the title coordination polymer, [Cu(1,4-BDOA)(2,2′-bipy)(H_2O)]$_n$ (where 1,4-BDOA^{2-} is benzene-1,4-dioxyacetate, $C_{10}H_8O_6$, and 2,2′-bipy is 2,2′-bipyridine, $C_{10}H_8N_2$), each Cu^{II} atom is six-coordinate and displays a distorted square-pyramidal geometry, with the basal plane capped by one very long semicoordinate Cu—O bond of 2.920 (3) Å. Adjacent Cu^{II} ions are bridged by carboxylate groups, resulting in a one-dimensional chain structure with a shortest Cu···Cu distance of 13.484 (3) Å. Furthermore, these chains are linked through hydrogen bonds and π–π stacking interactions to form a supramolecular network.

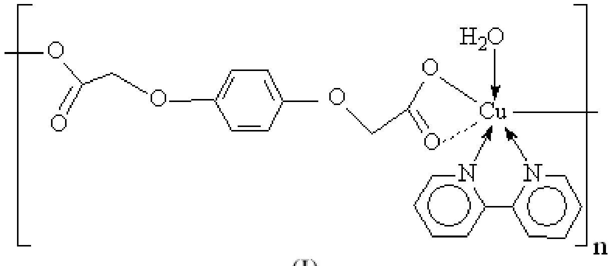
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.006 Å
R factor = 0.058
wR factor = 0.086
Data-to-parameter ratio = 15.6

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

Comment

In recent years, much interest has been focused on the self-assembly of supramolecular architectures, especially on coordination polymers with rigid organic aromatic carboxylic acid ligands, such as terephthalate and benzenetetracarboxylate (Franck *et al.*, 2002; Ye *et al.*, 2005). Phenylenedioxydiacetic acids (BDOAH$_2$), which have versatile binding modes, are regarded as excellent candidates for the construction of supramolecular architectures. Recently, we have reported the structures of some Cu^{II}, Zn^{II}, Co^{II} and Cd^{II} chain polymers incorporating 1,3- or 1,4-BDOA^{2-} groups (Gao, Li *et al.*, 2004; Gao *et al.*, 2004*a*,*b*,*c*). In the case of the one-dimensional chain polymers [Cu(1,3-BDOA)(2,2′-bipy)(H_2O)]$_n$, (II) (1,3-BDOA is benzene-1,3-dioxyacetate and 2,2′-bipy is 2,2′-bipyridine), the Cu^{II} atom shows a square-pyramidal configuration (Liu *et al.*, 2004). Here we have used 1,4-BDOAH$_2$ instead of 1,3-BDOAH$_2$ in the reaction and synthesized a new coordination polymer, [Cu(1,4-BDOA)(2,2′-bipy)(H_2O)]$_n$, (I), whose crystal structure is reported here.



(I)

As shown in Fig. 1, the Cu^{II} ion is six-coordinated by three carboxyl O atoms from two 1,4-BDOA^{2-} ligands, two N atoms from the 2,2′-bipy ligand and one water molecule; the local coordination environment around the Cu^{II} atom can be best described as a distorted square-pyramidal geometry, with the basal plane capped by one very long semicoordinate Cu1—O5

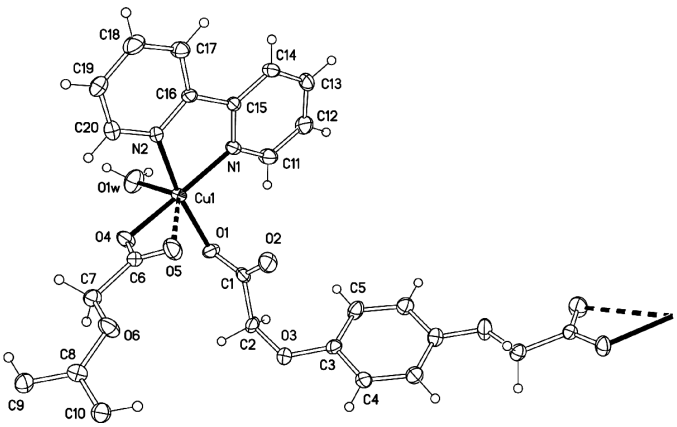


Figure 1
Part of the structure of (I), with displacement ellipsoids drawn at the 30% probability level. Weakly coordinated Cu1···O5 bonds are shown as dashed lines.

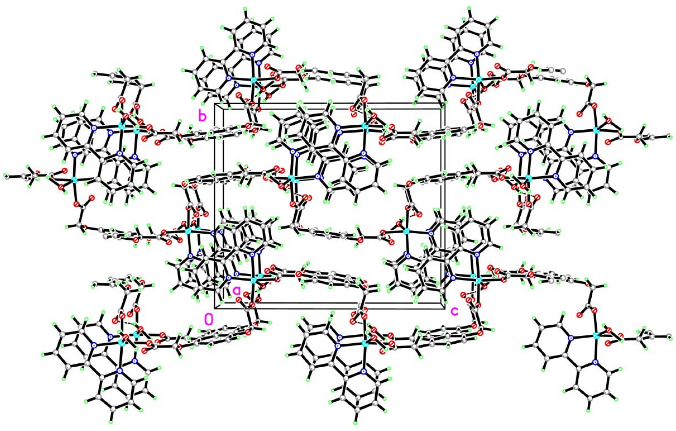


Figure 2
Packing diagram of (I), viewed down the *a* axis.

bond of 2.920 (3) Å (Sieroń *et al.*, 2002). Atoms O1, O4, N1 and N2 define the basal plane, and the Cu^{II} atom deviates by 0.16 (3) Å from that plane. A water molecule, O1*W*, occupies the apical site, with a Cu1—O1*W* bond distance of 2.241 (3) Å (Table 1). Adjacent Cu^{II} atoms are linked by 1,4-$BDOA^{2-}$ ligands into a one-dimensional chain structure. In the chain, the shortest Cu···Cu distance is 13.484 (3) Å, which is slightly longer than the value of 11.284 (3) Å in (II) (Liu *et al.*, 2004). With the help of the hydrogen-bonding and π–π stacking interactions between adjacent rings of the 2,2′-bipy ligands [centroid–centroid distance = 3.906 (3) Å], the polymeric chains are assembled to form a supramolecular network (Fig. 2 and Table 2).

Experimental

Benzene-1,4-dioxyacetic acid was prepared by the reaction of hydroquinol and chloroacetic acid (Mirci, 1990). The title complex was prepared by the addition of a stoichiometric amount of $Cu(Ac)_2 \cdot H_2O$ (4.00 g, 20 mmol) and 2,2′-bipy (3.12 g, 20 mmol) to a hot aqueous solution of 1,4-$BDOAH_2$ (4.52 g, 20 mmol); the pH was adjusted to 6 with NaOH solution (0.2 mol l^{-1}). The resulting solution was stirred for 30 min at room temperature and then filtered. Blue single crystals were isolated from the solution at room temperature over several days. Analysis calculated for $C_{20}H_{18}CuN_2O_7$: C 52.00, H 3.93, N 6.06%; found: C 51.79, H 3.80, N 6.01%.

Crystal data

$[Cu(C_{10}H_8O_6)(C_{10}H_8N_2)(H_2O)]$
M_r = 461.91
Orthorhombic, $P2_12_12_1$
a = 6.9836 (14) Å
b = 15.597 (3) Å
c = 17.506 (4) Å
V = 1906.8 (7) $Å^3$
Z = 4
D_x = 1.609 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 15 032 reflections
θ = 3.2–27.5°
μ = 1.19 mm^{-1}
T = 296 (2) K
Prism, blue
0.38 × 0.26 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.660, T_{max} = 0.814
16 530 measured reflections
4319 independent reflections
3071 reflections with $I > 2\sigma(I)$
R_{int} = 0.069
θ_{max} = 27.5°
h = −9 → 9
k = −19 → 20
l = −22 → 22

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.086
S = 1.03
4319 reflections
277 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 0.4933P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ <0.001
$\Delta\rho_{max}$ = 0.59 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.33 e $Å^{-3}$
Extinction correction: none
Absolute structure: Flack (1983). 1832 Friedel pairs
Flack parameter: 0.02 (2)

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.012 (3)	O1—C1	1.259 (5)
Cu1—N2	2.021 (3)	O2—C1	1.234 (5)
Cu1—O1	1.966 (3)	O4—C6	1.268 (5)
Cu1—O4	1.964 (3)	O5—C6	1.229 (5)
Cu1—O5	2.920 (3)		
N1—Cu1—N2	79.86 (14)	O1—Cu1—O1*W*	92.17 (12)
N1—Cu1—O1*W*	97.56 (14)	O4—Cu1—N1	169.96 (14)
N2—Cu1—O1*W*	98.42 (13)	O4—Cu1—N2	93.18 (14)
O1—Cu1—N1	94.78 (13)	O4—Cu1—O1	90.76 (14)
O1—Cu1—N2	168.65 (13)	O4—Cu1—O1*W*	90.58 (14)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2^{i}	0.84 (5)	2.10 (3)	2.874 (5)	152 (4)
O1*W*—H1*W*2···O5^{i}	0.84 (5)	2.11 (3)	2.843 (5)	145 (4)

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

C-bound H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, and were refined in the riding-model approximation. H atoms of water molecules were located in a difference map and refined with O—H and H···H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and $U_{iso}(H) = 1.5U_{eq}(O)$.

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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: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

The authors thank the National Natural Science Foundation of China (No. 20101003), the Scientific Fund of Remarkable Teachers of Heilongjiang Province (No. 1054 G036) and Heilongjiang University for supporting this work.

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