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catena-Poly[[aquabis(pyridine-κN)-copper(II)]-μ-2,2′-(*p*-phenylenedioxy)-diacetato-$\kappa^2 O$:O']

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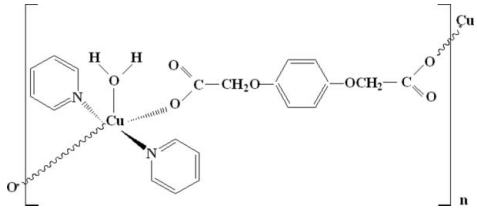
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.071; wR factor = 0.123; data-to-parameter ratio = 12.4.

In the title compound, $[Cu(C_{10}H_8O_6)(C_5H_5N)_2(H_2O)]_n$, the Cu atom is five-coordinated by two O atoms from two carboxylate groups of two different 2,2′-(*p*-phenylenedioxy)diacetate ligands, two N atoms from two pyridine molecules and one water O atom. The geometry is square-pyramidal with the water O atom occupying the apical position. The carboxylate group bridges adjacent Cu atoms, forming an infinite zigzag chain extending parallel to [001]. The chains are linked into layers by O—H···O hydrogen bonds. The Cu and water O atoms lie on special positions of site symmetry 2.

Related literature

For the isotypic zinc analog, see: Hong *et al.* (2005).



Experimental

Crystal data

$[Cu(C_{10}H_8O_6)(C_5H_5N)_2(H_2O)]$ M_r = 463.93
Monoclinic, $C2/c$
a = 15.363 (4) Å
b = 6.0888 (12) Å
c = 21.896 (6) Å
β = 103.67 (3)°
V = 1990.2 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.14 mm^{-1}
T = 298 K
0.12 × 0.11 × 0.09 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.875, T_{max} = 0.907
7227 measured reflections
1737 independent reflections
1096 reflections with $I > 2\sigma(I)$
R_{int} = 0.119

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.123
S = 1.08
1737 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1A···O2^{i}	0.81 (6)	1.87 (6)	2.677 (5)	174 (7)

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2000); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5029).

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supporting information

Acta Cryst. (2010). E**66**, m1283 [doi:10.1107/S1600536810036469]

catena-Poly[[aquabis(pyridine-κN)copper(II)]-μ-2,2′-(*p*-phenylenedioxy)-diacetato-$\kappa^2 O:O'$]

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S1. Comment

The metal-organic framework, which is formed by carboxylate ligand as the strut and transition metal as the node, has recently attracted more attentions owing to the potential applications of catalyst and H-storage. In this paper, flexible ligand-BDOA as the strut bridges the Cu cations to result in the formation of infinite zigzag chain of $[Cu(py)_2(H_2O)BDOA]_n$.

The asymmetrical unit of $[Cu(py)_2(H_2O)BDOA]_n$ (py=pyridine, BDOA=benzene-1,4-dioxyacetate) which is isostructural with of $[Zn(py)_2(H_2O)BDOA]_n$ (Hong, *et al.*, 2005), is composed of one half of Cu cation, one half of BDOA, one half of water molecule and one pyridine molecule (Fig.1). Five-coordinated Cu cation lies in the basal position of pyramid constructed by two O atoms from two carboxyl groups of two different BDOA, two nitrogen atoms of two pyridines and one water oxygen atom situated at the apical position. The bond distances of Cu—N, Cu—O and Cu—Ow are 2.109 (23) Å, 1.965 (35) Å and 2.192 (6) Å, respectively. The bond angles of O—Cu—O and N—Cu—O are 179.85 (14)° and 167.68 (18)°, respectively. Cu and water oxygen lie at 2-fold axis and BDOA at the inversion center.

The monodentate μ_2-BDOA bridges the adjacent Cu cations to form the infinite zigzag chain along (001) direction. The H-bonds of Ow—H···O (free oxygen of carboxyl) link the adjacent chains to two-dimensional layer (*bc* planar), which is packed by the ver dan Waals force (Fig.2).

S2. Experimental

(I) was synthesized under hydrothermal condition. In a typically route, H_2BDOA (0.22 g, 1 mmol) was dissolved in 10 ml deionized water under stirring, and then pyridine (1.6 ml, 20 mmol) and $Cu(Ac)_2{\cdot}3H_2O$ (0.235 g, 1 mmol) were added to a blue solution. After continuously stirred for 1 h, the solution with the molar ratio of H_2BDOA: 20py: $Cu(Ac)_2{\cdot}3H_2O$: 555H_2O was transferred into 23 ml autoclave and heated at 438 K for 5 days. After naturally cooling to room temperature, blue block product was collected by filtration as a single phase.

S3. Refinement

Water H atoms were located in a difference Fourier map and were refined with O—H = 0.82 (2) Å, H···H = 1.37 (2) Å and U_{iso}(H) = 1.2Ueq(O). The remaining H-atoms were placed in calculated positions (C—H (phenyl and pyridine ring) = 0.93 Å, C—H (methylene) = 0.97 Å) and were included in the refinement in the riding-model approximation, with U(H) = 1.2Ueq(C).

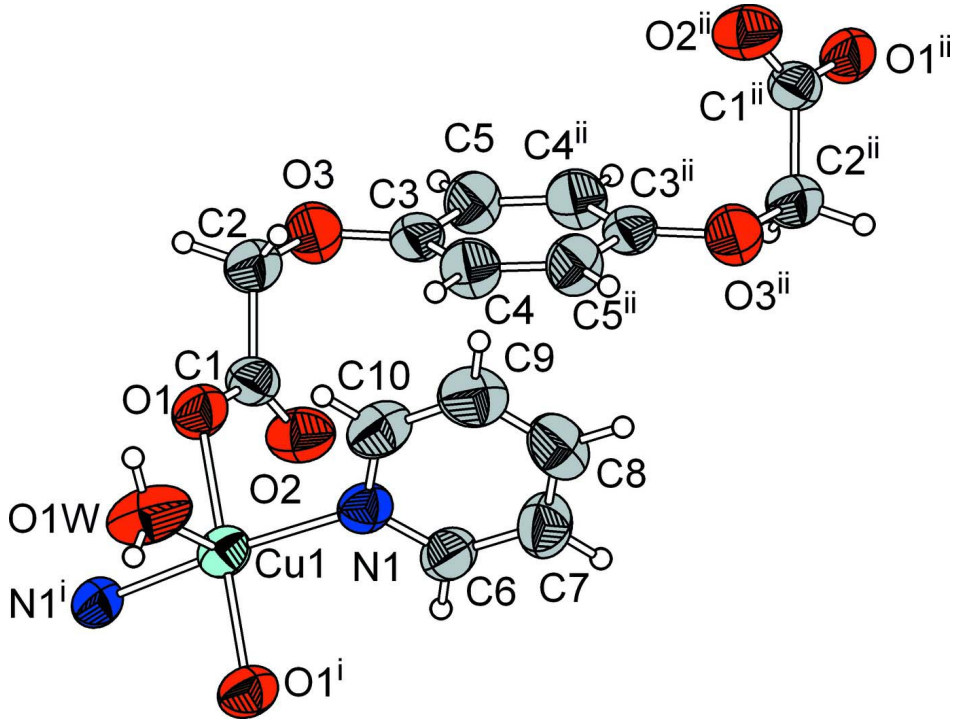

Figure 1

The unit cell of (I), showing the atomic labelling scheme and displacement ellipsoids at the 50% probability level. [Symmetry codes: (i) -*x*, *y*, 0.5 - *z*; (ii) -*x*, 1 - *y*, -*z*.]

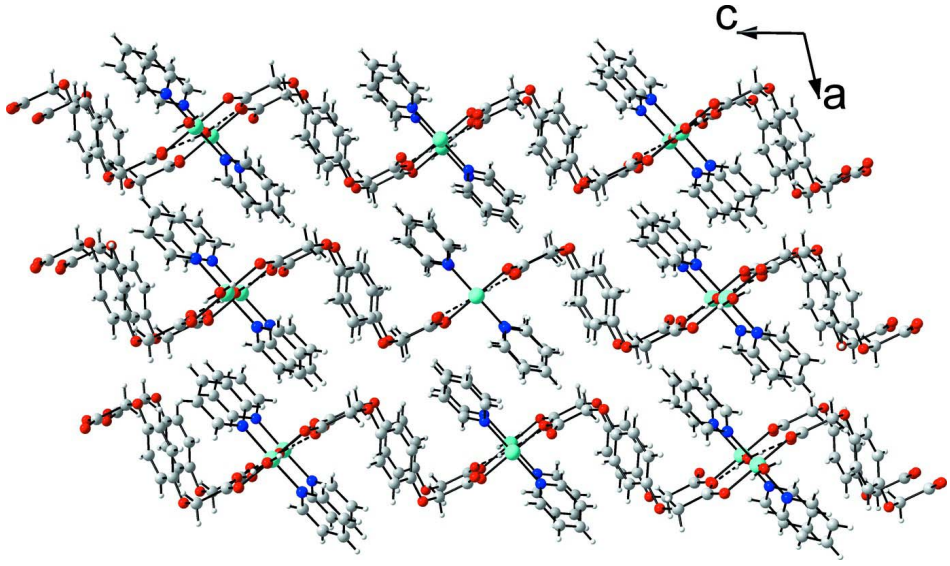

Figure 2

The ball-stick plot of (I), displaying the zigzag chain along (001) direction composed of briging the Cu cation with monodentate μ_2-BDOA. Cu is shown in the cyan, O in red, N in blue and C in grey.

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Crystal data

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Monoclinic, $C2/c$
Hall symbol: -C 2yc
a = 15.363 (4) Å
b = 6.0888 (12) Å
c = 21.896 (6) Å
β = 103.67 (3)°
V = 1990.2 (8) Å^3
Z = 4
$F(000)$ = 956
D_x = 1.548 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2000 reflections
θ = 3.6–25°
μ = 1.14 mm^{-1}
T = 298 K
Block, blue
0.12 × 0.11 × 0.09 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.00 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.875, T_{max} = 0.907
7227 measured reflections
1737 independent reflections
1096 reflections with $I > 2\sigma(I)$
R_{int} = 0.119
θ_{max} = 25.0°, θ_{min} = 3.6°
h = −18→18
k = −7→6
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.123
S = 1.08
1737 reflections
140 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0254P)^2 + 4.0919P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.
Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.0000	1.02668 (15)	0.2500	0.0480 (4)
O1	−0.0864 (2)	1.0271 (7)	0.16798 (16)	0.0584 (10)
O2	−0.0691 (3)	0.6662 (7)	0.15674 (17)	0.0679 (12)

O3	−0.1479 (3)	0.6794 (7)	0.03254 (17)	0.0656 (12)
C1	−0.0948 (4)	0.8473 (11)	0.1365 (2)	0.0506 (15)
C2	−0.1406 (4)	0.8781 (10)	0.0675 (2)	0.0581 (16)
H2A	−0.2001	0.9377	0.0643	0.070*
H2B	−0.1070	0.9840	0.0493	0.070*
C3	−0.0715 (4)	0.5975 (10)	0.0191 (2)	0.0528 (15)
C4	0.0125 (4)	0.6894 (10)	0.0344 (3)	0.0618 (17)
H4	0.0218	0.8182	0.0579	0.074*
C5	−0.0824 (4)	0.4048 (10)	−0.0158 (3)	0.0605 (17)
H5	−0.1385	0.3387	−0.0266	0.073*
N1	0.0988 (3)	0.9911 (8)	0.20420 (18)	0.0503 (12)
C6	0.1565 (4)	0.8241 (10)	0.2156 (3)	0.0571 (16)
H6	0.1512	0.7228	0.2463	0.068*
C7	0.2226 (4)	0.7939 (11)	0.1847 (3)	0.0681 (18)
H7	0.2605	0.6731	0.1937	0.082*
C8	0.2327 (4)	0.9417 (13)	0.1405 (3)	0.0713 (19)
H8	0.2787	0.9270	0.1198	0.086*
C9	0.1732 (5)	1.1140 (12)	0.1271 (3)	0.075 (2)
H9	0.1771	1.2156	0.0962	0.090*
C10	0.1086 (4)	1.1333 (10)	0.1598 (3)	0.0659 (18)
H10	0.0693	1.2514	0.1508	0.079*
O1W	0.0000	1.3867 (10)	0.2500	0.085 (2)
H1A	0.023 (5)	1.463 (10)	0.280 (3)	0.102*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0449 (6)	0.0454 (6)	0.0508 (6)	0.000	0.0055 (4)	0.000
O1	0.047 (2)	0.067 (3)	0.055 (2)	0.003 (2)	0.0017 (18)	−0.007 (2)
O2	0.082 (3)	0.057 (3)	0.059 (3)	0.000 (2)	0.006 (2)	0.007 (2)
O3	0.052 (3)	0.080 (3)	0.062 (2)	−0.005 (2)	0.009 (2)	−0.016 (2)
C1	0.040 (4)	0.069 (5)	0.042 (3)	−0.005 (3)	0.008 (3)	0.001 (3)
C2	0.055 (4)	0.064 (4)	0.052 (3)	0.004 (3)	0.005 (3)	−0.001 (3)
C3	0.043 (4)	0.070 (4)	0.042 (3)	−0.001 (3)	0.004 (3)	−0.002 (3)
C4	0.057 (5)	0.065 (4)	0.060 (4)	−0.010 (3)	0.008 (3)	−0.015 (3)
C5	0.042 (4)	0.072 (4)	0.067 (4)	−0.012 (3)	0.013 (3)	−0.006 (3)
N1	0.042 (3)	0.057 (3)	0.048 (3)	−0.005 (3)	0.004 (2)	0.001 (2)
C6	0.051 (4)	0.062 (4)	0.057 (4)	0.005 (3)	0.010 (3)	0.011 (3)
C7	0.054 (5)	0.073 (5)	0.081 (5)	0.005 (4)	0.024 (4)	0.006 (4)
C8	0.049 (4)	0.103 (6)	0.066 (4)	−0.026 (4)	0.020 (3)	−0.020 (4)
C9	0.063 (5)	0.093 (5)	0.070 (4)	−0.018 (4)	0.018 (4)	0.017 (4)
C10	0.053 (4)	0.069 (4)	0.070 (4)	−0.004 (3)	0.004 (3)	0.015 (4)
O1W	0.114 (6)	0.041 (4)	0.078 (5)	0.000	−0.021 (4)	0.000

Geometric parameters (Å, º)

Cu1—O1	1.964 (3)	C4—H4	0.9300
Cu1—O1^{i}	1.964 (3)	C5—C4^{ii}	1.362 (8)

Cu1—N1	2.019 (4)	C5—H5	0.9300
Cu1—N1^{i}	2.019 (4)	N1—C6	1.333 (7)
Cu1—O1W	2.192 (6)	N1—C10	1.338 (7)
O1—C1	1.284 (6)	C6—C7	1.359 (8)
O2—C1	1.219 (6)	C6—H6	0.9300
O3—C3	1.370 (6)	C7—C8	1.357 (8)
O3—C2	1.422 (6)	C7—H7	0.9300
C1—C2	1.520 (7)	C8—C9	1.377 (9)
C2—H2A	0.9700	C8—H8	0.9300
C2—H2B	0.9700	C9—C10	1.357 (8)
C3—C4	1.373 (7)	C9—H9	0.9300
C3—C5	1.388 (8)	C10—H10	0.9300
C4—C5^{ii}	1.362 (8)	O1W—H1A	0.81 (6)

O1—Cu1—O1^{i}	179.8 (3)	C5^{ii}—C4—H4	119.4
O1—Cu1—N1	88.32 (15)	C3—C4—H4	119.4
O1^{i}—Cu1—N1	91.70 (15)	C4^{ii}—C5—C3	121.3 (6)
O1—Cu1—N1^{i}	91.70 (15)	C4^{ii}—C5—H5	119.4
O1^{i}—Cu1—N1^{i}	88.32 (15)	C3—C5—H5	119.4
N1—Cu1—N1^{i}	167.7 (3)	C6—N1—C10	116.5 (5)
O1—Cu1—O1W	89.92 (13)	C6—N1—Cu1	122.2 (4)
O1^{i}—Cu1—O1W	89.92 (13)	C10—N1—Cu1	121.3 (4)
N1—Cu1—O1W	96.16 (14)	N1—C6—C7	123.5 (6)
N1^{i}—Cu1—O1W	96.16 (14)	N1—C6—H6	118.3
C1—O1—Cu1	116.8 (4)	C7—C6—H6	118.3
C3—O3—C2	117.5 (5)	C8—C7—C6	119.4 (6)
O2—C1—O1	126.4 (5)	C8—C7—H7	120.3
O2—C1—C2	120.4 (5)	C6—C7—H7	120.3
O1—C1—C2	113.1 (5)	C7—C8—C9	118.3 (6)
O3—C2—C1	113.0 (5)	C7—C8—H8	120.8
O3—C2—H2A	109.0	C9—C8—H8	120.8
C1—C2—H2A	109.0	C10—C9—C8	119.0 (6)
O3—C2—H2B	109.0	C10—C9—H9	120.5
C1—C2—H2B	109.0	C8—C9—H9	120.5
H2A—C2—H2B	107.8	N1—C10—C9	123.3 (6)
O3—C3—C4	127.1 (6)	N1—C10—H10	118.4
O3—C3—C5	115.3 (5)	C9—C10—H10	118.4
C4—C3—C5	117.6 (6)	Cu1—O1W—H1A	125 (5)
C5^{ii}—C4—C3	121.1 (6)		

N1—Cu1—O1—C1	66.8 (4)	O1^{i}—Cu1—N1—C6	56.9 (4)
N1^{i}—Cu1—O1—C1	−100.9 (4)	N1^{i}—Cu1—N1—C6	−33.0 (4)
O1W—Cu1—O1—C1	162.9 (4)	O1W—Cu1—N1—C6	147.0 (4)
Cu1—O1—C1—O2	15.7 (8)	O1—Cu1—N1—C10	55.6 (4)
Cu1—O1—C1—C2	−163.2 (3)	O1^{i}—Cu1—N1—C10	−124.3 (4)
C3—O3—C2—C1	−73.6 (6)	N1^{i}—Cu1—N1—C10	145.9 (4)
O2—C1—C2—O3	−0.3 (8)	O1W—Cu1—N1—C10	−34.1 (4)
O1—C1—C2—O3	178.6 (5)	C10—N1—C6—C7	−0.1 (8)

C2—O3—C3—C4	−1.8 (8)	Cu1—N1—C6—C7	178.8 (4)
C2—O3—C3—C5	−179.3 (4)	N1—C6—C7—C8	1.3 (10)
O3—C3—C4—C5^{ii}	−177.2 (5)	C6—C7—C8—C9	−2.2 (9)
C5—C3—C4—C5^{ii}	0.3 (9)	C7—C8—C9—C10	2.0 (9)
O3—C3—C5—C4^{ii}	177.5 (5)	C6—N1—C10—C9	−0.1 (8)
C4—C3—C5—C4^{ii}	−0.3 (9)	Cu1—N1—C10—C9	−179.0 (5)
O1—Cu1—N1—C6	−123.2 (4)	C8—C9—C10—N1	−0.9 (10)

Symmetry codes: (i) −*x*, *y*, −*z*+1/2; (ii) −*x*, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*A*···O2^{iii}	0.81 (6)	1.87 (6)	2.677 (5)	174 (7)

Symmetry code: (iii) −*x*, *y*+1, −*z*+1/2.