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catena-Poly[[diaquacopper(II)]-μ-2,2′-bipyridine-3,3′-dicarboxylate]

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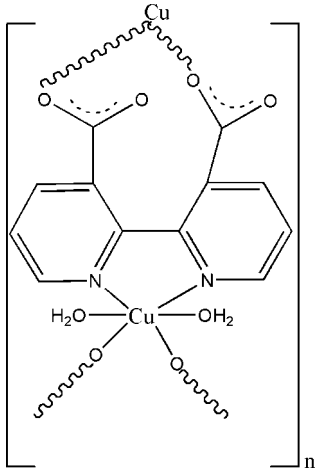
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.130; data-to-parameter ratio = 10.0.

In the title compound, $[Cu(C_{12}H_6N_2O_4)(H_2O)_2]_n$, the 2,2′-bipyridine-3,3′-dicarboxylate (dcbp) dianion lies on a twofold rotation axis. The Cu atom also lies on this axis and is coordinated by two N atoms and two O atoms of two bridging dcbp ligands in the equatorial plane. Two aqua ligands complete the distorted *cis*-CuN_2O_4 octahedral coordination of the Cu atom. O—H···O hydrogen bonds help to stabilize the structure.

Related literature

For related literature, see: Starova *et al.* (2007).



Experimental

Crystal data

$[Cu(C_{12}H_6N_2O_4)(H_2O)_2]$
M_r = 341.76
Monoclinic, $C2/c$
a = 11.3254 (15) Å
b = 7.8829 (10) Å
c = 13.1264 (17) Å
β = 100.519 (2)°
V = 1152.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.93 mm^{-1}
T = 298 (2) K
0.31 × 0.19 × 0.14 mm

Data collection

Bruker APEX-II CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.586, T_{max} = 0.774
2925 measured reflections
1044 independent reflections
1007 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.130
S = 0.86
1044 reflections
104 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N1	2.099 (3)	Cu1—O1	2.113 (2)
Cu1—O2^{i}	2.111 (2)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1WB···O3^{ii}	0.86 (3)	1.87 (2)	2.647 (3)	150 (4)
O1—H1WA···O3^{iii}	0.86 (2)	1.90 (3)	2.744 (3)	167 (4)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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, 2004); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2612).

References

Bruker (2004). *APEX2* (Version 6.12) and *SMART* (Version 6.12). Bruker AXS Inc, Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.
Starova, G. L., Denisova, A. S. & Dem'yanchuk, E. M. (2007). *J. Mol. Struct.* **830**, 139–142.

supplementary materials

Acta Cryst. (2007). E**63**, m3155 [**doi:10.1107/S1600536807060229**]

catena-Poly[[diaquacopper(II)]-μ-2,2'-bipyridine-3,3'-dicarboxylate]

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Comment

Transition metal complexes with 2,2'-bipyridine derivatives can serve as models for the study of excited state dynamics. In addition, they are of interest for the development of light-energy conversion devices and optical sensors. One of the simplest carbonyl-containing derivatives of 2,2'-bipyridine is 3,3'-dicarboxy-2,2'-bipyridine (dcbp) which has two available centres for complexation: the nitrogen atoms of bipyridine fragment and the oxygen atoms of the carboxylic groups. (Starova *et al.*, 2007). In this paper, we report the synthesis and crystal structure of the title complex, (I), (Fig. 1).

In (I), the copper atom (site symmetry 2) is bridged by two N atoms and two O atoms of two dcbp ligands in the basal plane. The remaining positions are occupied by two water molecules and complete the octahedral coordination sphere of Cu atom (Table 1). The dcbp ligands link the neighboring Cu ions *via* two carboxlate groups forming an infinite chain.

The structure of (I) is completed by O—H···O hydrogen bonds (Table 2).

Experimental

$CuCl_2$ (0.011 g, 0.0095 mmol), H_2dcbp (0.013 g, 0.011 mmol) and NaOH (0.047 g, 0.12 mmol), were added to a mixed solvent of ethanol and acetonitrile, and the mixture was heated for five hours under reflux with stirring. The resultant was then filtered to give a solution which was infiltrated by diethyl ether in a closed vessel. After one week, blue blocks of (I) were recovered.

Refinement

The H atoms (pyridine ring) were placed in calculated positions [Csp^2—H = 0.93 Å] and refined as riding with U_{iso}(H) = 1.2U_{eq}(C). The water H atoms were found in a dfference map (O—H = 0.86 Å), with U_{iso}(H) = 1.5U_{eq}(C).

Figures

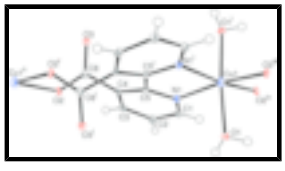

Fig. 1. A fragemnt of the chain structure of (I) showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms). Symmetry codes: (i) 1 − *x*, *y*, 1/2 − *z*; (ii) *x*, *y* + 1, *z*; (iii) 1 − *x*, *y* − 1, 1/2 − *z*; (iv) *x*, *y* − 1, *z*.

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Crystal data

$[Cu(C_{12}H_6N_2O_4)(H_2O)_2]$ F_{000} = 692

M_r = 341.76	D_x = 1.970 Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 1044 reflections
a = 11.3254 (15) Å	θ = 3.2–25.2°
b = 7.8829 (10) Å	μ = 1.93 mm^{-1}
c = 13.1264 (17) Å	T = 298 (2) K
β = 100.519 (2)°	Block, blue
V = 1152.2 (3) Å^3	0.31 × 0.19 × 0.14 mm
Z = 4	

Data collection

Bruker APEX-II CCD diffractometer	1044 independent reflections
Radiation source: fine-focus sealed tube	1007 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
Detector resolution: 0 pixels mm^{-1}	θ_{max} = 25.2°
T = 298(2) K	θ_{min} = 3.2°
φ and ω scan	h = −13→11
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	k = −9→9
T_{min} = 0.586, T_{max} = 0.774	l = −15→15
2925 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.038	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.130	$w = 1/[\sigma^2(F_o^2) + (0.1078P)^2 + 11.1055P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.86	$(\Delta/\sigma)_{max} < 0.001$
1044 reflections	$\Delta\rho_{max}$ = 0.60 e Å^{-3}
104 parameters	$\Delta\rho_{min}$ = −0.44 e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
O2	0.4605 (2)	1.0082 (3)	0.13881 (18)	0.0102 (5)
C6	0.5228 (3)	0.8739 (4)	0.1493 (2)	0.0089 (7)
Cu1	0.5000	0.20313 (7)	0.2500	0.0146 (3)
O1	0.3250 (2)	0.1907 (3)	0.2842 (2)	0.0119 (6)
O3	0.6348 (2)	0.8655 (3)	0.17267 (19)	0.0129 (6)
N1	0.4346 (2)	0.4120 (4)	0.1575 (2)	0.0089 (6)
C1	0.3728 (3)	0.3938 (4)	0.0607 (3)	0.0113 (7)
H1	0.3488	0.2856	0.0372	0.014*
C2	0.3433 (3)	0.5301 (4)	−0.0057 (3)	0.0126 (7)
H2	0.2944	0.5164	−0.0702	0.015*
C3	0.3893 (3)	0.6873 (4)	0.0274 (3)	0.0104 (7)
H3	0.3751	0.7802	−0.0168	0.012*
C4	0.4571 (3)	0.7073 (4)	0.1271 (3)	0.0076 (7)
C5	0.4708 (3)	0.5671 (4)	0.1933 (2)	0.0077 (7)
H1WA	0.265 (2)	0.232 (4)	0.242 (3)	0.022 (12)*
H1WB	0.311 (3)	0.088 (2)	0.301 (3)	0.027 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0115 (12)	0.0049 (12)	0.0126 (12)	0.0014 (9)	−0.0022 (9)	−0.0005 (9)
C6	0.0141 (16)	0.0069 (16)	0.0057 (14)	−0.0012 (13)	0.0017 (12)	0.0001 (12)
Cu1	0.0149 (4)	0.0106 (4)	0.0174 (4)	0.000	0.0007 (3)	0.000
O1	0.0077 (12)	0.0093 (13)	0.0185 (14)	0.0013 (9)	0.0018 (10)	0.0032 (9)
O3	0.0094 (12)	0.0088 (12)	0.0193 (13)	0.0003 (9)	−0.0005 (10)	0.0003 (10)
N1	0.0085 (13)	0.0074 (14)	0.0101 (14)	0.0003 (11)	−0.0001 (11)	−0.0008 (11)
C1	0.0094 (16)	0.0097 (16)	0.0137 (16)	−0.0015 (12)	−0.0003 (13)	−0.0027 (13)
C2	0.0117 (16)	0.0139 (18)	0.0111 (16)	0.0008 (14)	−0.0008 (13)	−0.0030 (13)
C3	0.0088 (17)	0.0122 (17)	0.0094 (17)	0.0030 (12)	−0.0006 (13)	−0.0002 (12)
C4	0.0068 (16)	0.0058 (17)	0.0102 (17)	0.0020 (11)	0.0017 (13)	−0.0021 (11)
C5	0.0068 (15)	0.0074 (15)	0.0087 (17)	−0.0001 (12)	0.0013 (12)	−0.0019 (12)

Geometric parameters (Å, °)

O2—C6	1.266 (4)	O1—H1WB	0.86 (2)
O2—Cu1^{i}	2.111 (2)	N1—C1	1.342 (5)
C6—O3	1.250 (4)	N1—C5	1.346 (4)
C6—C4	1.511 (4)	C1—C2	1.385 (5)
Cu1—N1^{ii}	2.099 (3)	C1—H1	0.9300

Cu1—N1	2.099 (3)	C2—C3	1.383 (5)
Cu1—O2^{iii}	2.111 (2)	C2—H2	0.9300
Cu1—O2^{iv}	2.111 (2)	C3—C4	1.400 (5)
Cu1—O1	2.113 (2)	C3—H3	0.9300
Cu1—O1^{ii}	2.113 (2)	C4—C5	1.397 (5)
O1—H1WA	0.86 (3)	C5—C5^{ii}	1.516 (6)
C6—O2—Cu1^{i}	119.4 (2)	Cu1—O1—H1WB	108 (3)
O3—C6—O2	126.3 (3)	H1WA—O1—H1WB	111 (3)
O3—C6—C4	116.3 (3)	C1—N1—C5	120.0 (3)
O2—C6—C4	117.4 (3)	C1—N1—Cu1	122.1 (2)
N1^{ii}—Cu1—N1	76.66 (15)	C5—N1—Cu1	117.2 (2)
N1^{ii}—Cu1—O2^{iii}	168.28 (10)	N1—C1—C2	122.5 (3)
N1—Cu1—O2^{iii}	99.40 (10)	N1—C1—H1	118.8
N1^{ii}—Cu1—O2^{iv}	99.40 (10)	C2—C1—H1	118.8
N1—Cu1—O2^{iv}	168.28 (10)	C3—C2—C1	117.6 (3)
O2^{iii}—Cu1—O2^{iv}	86.52 (13)	C3—C2—H2	121.2
N1^{ii}—Cu1—O1	99.16 (10)	C1—C2—H2	121.2
N1—Cu1—O1	85.03 (10)	C2—C3—C4	120.4 (3)
O2^{iii}—Cu1—O1	91.41 (10)	C2—C3—H3	119.8
O2^{iv}—Cu1—O1	84.71 (9)	C4—C3—H3	119.8
N1^{ii}—Cu1—O1^{ii}	85.03 (10)	C5—C4—C3	118.1 (3)
N1—Cu1—O1^{ii}	99.16 (10)	C5—C4—C6	125.0 (3)
O2^{iii}—Cu1—O1^{ii}	84.71 (9)	C3—C4—C6	116.4 (3)
O2^{iv}—Cu1—O1^{ii}	91.41 (9)	N1—C5—C4	120.7 (3)
O1—Cu1—O1^{ii}	174.69 (13)	N1—C5—C5^{ii}	113.15 (19)
Cu1—O1—H1WA	121 (3)	C4—C5—C5^{ii}	126.1 (2)

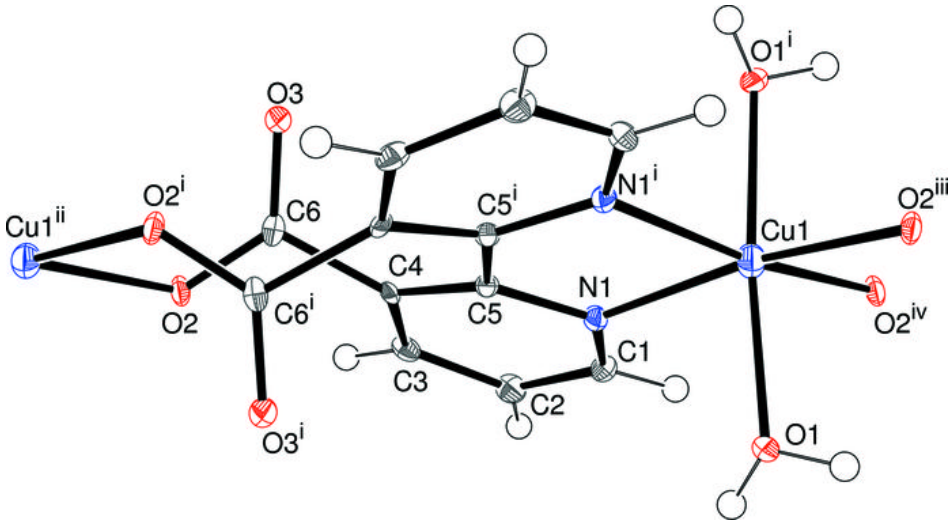
Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*+1, *y*, −*z*+1/2; (iii) *x*, *y*−1, *z*; (iv) −*x*+1, *y*−1, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1WB···O3^{iv}	0.86 (3)	1.87 (2)	2.647 (3)	150 (4)
O1—H1WA···O3^{v}	0.86 (2)	1.90 (3)	2.744 (3)	167 (4)

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

Fig. 1


O1i
O3
O2i
C6
C5i
N1i
Cu1ii
Cu1
O2iii
C4
N1
C5
O2
C6i
O2iv
C1
C3
C2
O3i
O1