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catena-Poly[[[diaquacopper(II)]-{μ-4,4′-[1,4-phenylenebis(methyleneimino)]-dibenzoato}] monohydrate]

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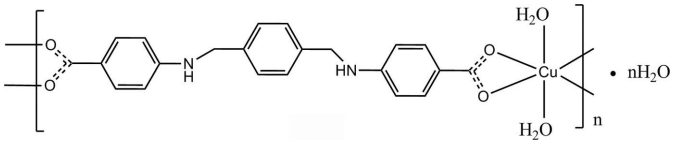
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; R factor = 0.043; wR factor = 0.140; data-to-parameter ratio = 17.2.

The asymmetric unit of the title polymeric compound, $\{[Cu(C_{22}H_{18}N_2O_4)(H_2O)_2]\cdot H_2O\}_n$, contains a Cu ion situated on an inversion center, half of a centrosymmetric 4,4′-[1,4-phenylenebis(methyleneimino)]dibenzoate ligand, a coordinated water molecule in a general position and an uncoordinated water molecule situated on a twofold rotation axis. The distorted octahedral coordination geometry of the Cu^{II} ion is formed by six O atoms. The –NH– groups of the ligand are involved in intramolecular N—H···O hydrogen bonds, while the water molecules participate in the formation of a three-dimensional supramolecular framework *via* intermolecular O—H···O hydrogen bonds.

Related literature

For properties of 4,4′-(1,4-phenylenebis(methylene))bis(azanediyl)dibenzoic acid and its ramifications, see: Yamaguchi *et al.* (1991); Imhof & Göbel (2000). For supramolecular networks in related structures, see: Jing *et al.* (2006).



Experimental

Crystal data

$[Cu(C_{22}H_{18}N_2O_4)(H_2O)_2]\cdot H_2O$
M_r = 491.98
Monoclinic, $P2/c$
a = 16.127 (6) Å
b = 5.1535 (17) Å
c = 13.405 (8) Å
β = 92.76 (2)°
V = 1112.8 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.03 mm^{-1}
T = 291 (2) K
0.09 × 0.08 × 0.07 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.913, T_{max} = 0.932
10220 measured reflections
2534 independent reflections
2008 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.140
S = 1.03
2534 reflections
147 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—O1	1.992 (3)	Cu1—O3	2.582 (2)
Cu1—O2	2.006 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3	0.84	2.00	2.676 (3)	137
O1—H1A···O3^{i}	0.85	2.17	3.011 (3)	174
O1—H1B···O4^{ii}	0.85	2.28	3.104 (3)	164
O4—H4A···O2^{iii}	0.85	2.03	2.855 (3)	163

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+1, -y, -z+2$; (iii) $x, y+1, z$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-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: *PLATON* (Spek, 2003); 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: CV2427).

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catena-Poly[[[diaquacopper(II)]-{μ-4,4′-[1,4-phenylenebis(methylene-imino)]dibenzoato}] monohydrate]

Qiu-sheng Wang and Jie Ouyang

S1. Comment

In recent years, 4,4′-(1,4-phenylenebis(methylene))bis(azanediyl)dibenzoic acid and its ramifications have become an area of interest owing to their various properties (Yamaguchi *et al.*, 1991; Imhof & Göbel, 2000). They are also used for building up supramolecular networks through hydrogen bonds (Jing *et al.*, 2006). Of special interest are the low-dimensional structural motifs related with highly anisotropic physical properties. Here we report the crystal structure of the title compound, (I).

For the title polymeric compound, (I), structure determination revealed a presence in the asymmetric unit of a half of centrosymmetric 4,4′-(1,4-phenylenebis(methylene))bis(azanediyl)dibenzoic ligand, one Cu ion lies on the inversion ctnter, one coordinated water molecule locates on the twofold axis and one lattice water molecule locates in the general positon. The Cu ion is coordinated by six oxygen atoms with four of which from 4,4′-(1,4-phenylenebis(methylene))bis-(azanediyl)dibenzoic ligand and the other two from water moleculers into a distorted octahedral geometry (Table 1). The neighbouring Cu ions are linked by 4,4′-(1,4-phenylenebis(methylene))bis(azanediyl)dibenzoic ligand to form an infinite plolymeric zigzag chain (Fig. 1). The amino groups of the ligand are involved in intramolecular N—H···O hydrogen bonds, wihle water molecules participate in formation of three-dimensional supramolecular framework via intermolecular O—H···O hydrogen bonds (Table 2).

S2. Experimental

The 10 ml aqueous solution of $CuCl_2.2H_2O$ (0.855 g, 5 mmol) was droped into a 10 ml DMF soution of 4,4′-(1,4-phenyl-enebis(methylene))bis(azanediyl)dibenzoic acid (1.882 g, 5 mmol). The mixture was stirred for half an hour. The resultant solution was filtered, and the filtrate was allowed to stand at room temperature for one week, to generate blue block crystals.

S3. Refinement

C-bound H atoms were geometrically positioned (C-H 0.93-0.97 Å) and treated as riding on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C) Water H atoms were positioned geometrically with O—H = 0.85 Å and U_{iso}(H) = 1.2U_{eq}(O). The N-bound H atom was located on a difference Fourier map, but placed in idealized position (N-H 0.84 Å) and refined as ridinh with U_{iso}(H) = 1.5U_{eq}(N).

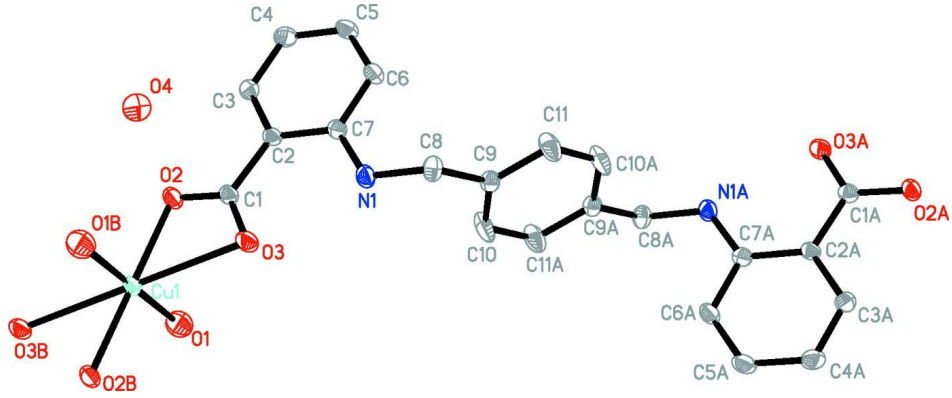

Figure 1

A portion of the polymeric chain in (I) with the atom numbering and 30% probalility displacement ellipsoids [symmetry codes: (A) 2-*x*, 1-*y*, 2-*z*; (B) 1-*x*, -*y*, 2-*z*]

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Crystal data

$[Cu(C_{22}H_{18}N_2O_4)(H_2O)_2]\cdot H_2O$
$M_r = 491.98$
Monoclinic, *P*2/*c*
Hall symbol: -P 2yc
$a = 16.127\ (6)$ Å
$b = 5.1535\ (17)$ Å
$c = 13.405\ (8)$ Å
$\beta = 92.76\ (2)°$
$V = 1112.8\ (8)$ Å^3
$Z = 2$
$F(000) = 510$
$D_x = 1.468$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7833 reflections
$\theta = 3.1–27.5°$
$\mu = 1.03$ mm^{-1}
$T = 291$ K
Block, blue
0.09 × 0.08 × 0.07 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.913$, $T_{max} = 0.932$
10220 measured reflections
2534 independent reflections
2008 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -20\rightarrow20$
$k = -6\rightarrow6$
$l = -17\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.140$
$S = 1.03$
2534 reflections
147 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0854P)^2 + 0.6974P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.63113 (17)	0.1232 (5)	0.8986 (2)	0.0276 (6)
C2	0.69938 (16)	0.1294 (5)	0.82720 (19)	0.0253 (5)
C3	0.69767 (18)	−0.0493 (6)	0.7480 (2)	0.0312 (6)
H3	0.6542	−0.1676	0.7419	0.037*
C4	0.7583 (2)	−0.0552 (7)	0.6790 (2)	0.0383 (7)
H4	0.7554	−0.1729	0.6264	0.046*
C5	0.82372 (19)	0.1176 (7)	0.6898 (2)	0.0374 (7)
H5	0.8653	0.1143	0.6441	0.045*
C6	0.82859 (18)	0.2944 (6)	0.7668 (2)	0.0333 (6)
H6	0.8733	0.4083	0.7724	0.040*
C7	0.76652 (16)	0.3050 (5)	0.8376 (2)	0.0264 (5)
C8	0.83674 (18)	0.6789 (5)	0.9238 (2)	0.0328 (6)
H8A	0.8186	0.8126	0.9687	0.039*
H8B	0.8427	0.7584	0.8590	0.039*
C9	0.92123 (18)	0.5803 (6)	0.9623 (2)	0.0287 (6)
C10	0.9299 (2)	0.3842 (8)	1.0310 (3)	0.0506 (9)
H10	0.8826	0.3031	1.0530	0.061*
C11	0.9926 (2)	0.6965 (7)	0.9314 (3)	0.0484 (9)
H11	0.9888	0.8303	0.8848	0.058*
Cu1	0.5000	0.0000	1.0000	0.02769 (18)
N1	0.77292 (15)	0.4809 (5)	0.91439 (19)	0.0326 (5)
H1	0.7305	0.4913	0.9484	0.049*
O1	0.56996 (16)	−0.2511 (5)	1.07956 (19)	0.0517 (6)
H1A	0.5868	−0.3765	1.0447	0.062*
H1B	0.5446	−0.3136	1.1282	0.062*
O2	0.57429 (13)	−0.0498 (4)	0.88572 (16)	0.0337 (5)
O3	0.62970 (13)	0.2785 (4)	0.97072 (15)	0.0371 (5)
O4	0.5000	0.5811 (7)	0.7500	0.0450 (8)
H4A	0.5284	0.6994	0.7798	0.054*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0219 (13)	0.0338 (14)	0.0275 (14)	0.0043 (11)	0.0040 (10)	0.0018 (11)
C2	0.0218 (13)	0.0306 (14)	0.0237 (13)	0.0036 (10)	0.0039 (10)	0.0019 (10)
C3	0.0263 (14)	0.0380 (15)	0.0293 (15)	0.0004 (11)	0.0023 (11)	−0.0025 (11)

C4	0.0366 (17)	0.0494 (18)	0.0294 (15)	0.0018 (14)	0.0073 (12)	−0.0090 (12)
C5	0.0325 (16)	0.0504 (18)	0.0303 (15)	0.0016 (14)	0.0114 (12)	0.0013 (13)
C6	0.0259 (14)	0.0403 (16)	0.0345 (15)	−0.0032 (12)	0.0080 (11)	0.0032 (12)
C7	0.0222 (13)	0.0308 (13)	0.0264 (13)	0.0051 (10)	0.0016 (10)	0.0035 (10)
C8	0.0263 (14)	0.0307 (14)	0.0410 (16)	0.0006 (11)	−0.0027 (11)	−0.0008 (12)
C9	0.0269 (14)	0.0273 (12)	0.0318 (14)	−0.0003 (11)	0.0005 (11)	−0.0023 (11)
C10	0.0249 (16)	0.057 (2)	0.070 (2)	−0.0083 (15)	0.0041 (15)	0.0301 (18)
C11	0.0311 (16)	0.053 (2)	0.061 (2)	−0.0044 (15)	0.0001 (15)	0.0326 (17)
Cu1	0.0237 (3)	0.0304 (3)	0.0297 (3)	−0.00293 (19)	0.00892 (18)	−0.00458 (18)
N1	0.0225 (12)	0.0392 (14)	0.0365 (13)	−0.0030 (10)	0.0055 (10)	−0.0070 (10)
O1	0.0498 (15)	0.0521 (14)	0.0537 (15)	0.0052 (12)	0.0086 (12)	−0.0021 (11)
O2	0.0267 (10)	0.0391 (11)	0.0361 (11)	−0.0065 (8)	0.0102 (8)	−0.0065 (8)
O3	0.0335 (11)	0.0444 (12)	0.0346 (11)	−0.0045 (9)	0.0133 (8)	−0.0111 (9)
O4	0.048 (2)	0.0425 (16)	0.0444 (19)	0.000	0.0024 (15)	0.000

Geometric parameters (Å, º)

C1—O3	1.257 (3)	C9—C10	1.370 (4)
C1—O2	1.284 (4)	C9—C11	1.379 (4)
C1—C2	1.493 (4)	C10—C11^{i}	1.389 (5)
C2—C3	1.405 (4)	C10—H10	0.9300
C2—C7	1.413 (4)	C11—C10^{i}	1.389 (5)
C3—C4	1.378 (4)	C11—H11	0.9300
C3—H3	0.9300	Cu1—O1^{ii}	1.992 (3)
C4—C5	1.383 (5)	Cu1—O1	1.992 (3)
C4—H4	0.9300	Cu1—O2	2.006 (2)
C5—C6	1.376 (4)	Cu1—O2^{ii}	2.006 (2)
C5—H5	0.9300	Cu1—O3	2.582 (2)
C6—C7	1.413 (4)	Cu1—O3^{ii}	2.582 (2)
C6—H6	0.9300	Cu1—C1^{ii}	2.646 (3)
C7—N1	1.372 (4)	N1—H1	0.8420
C8—N1	1.450 (4)	O1—H1A	0.8500
C8—C9	1.521 (4)	O1—H1B	0.8500
C8—H8A	0.9700	O4—H4A	0.8500
C8—H8B	0.9700		
O3—C1—O2	120.4 (3)	C9—C11—C10^{i}	120.7 (3)
O3—C1—C2	121.4 (3)	C9—C11—H11	119.7
O2—C1—C2	118.2 (2)	C10^{i}—C11—H11	119.7
C3—C2—C7	118.8 (2)	O1^{ii}—Cu1—O1	180.00 (13)
C3—C2—C1	118.8 (2)	O1^{ii}—Cu1—O2	91.02 (10)
C7—C2—C1	122.4 (2)	O1—Cu1—O2	88.98 (10)
C4—C3—C2	122.2 (3)	O1^{ii}—Cu1—O2^{ii}	88.98 (10)
C4—C3—H3	118.9	O1—Cu1—O2^{ii}	91.02 (10)
C2—C3—H3	118.9	O2—Cu1—O2^{ii}	180.000 (1)
C3—C4—C5	118.5 (3)	O1^{ii}—Cu1—O3	89.98 (10)
C3—C4—H4	120.7	O1—Cu1—O3	90.02 (10)
C5—C4—H4	120.7	O2—Cu1—O3	55.75 (7)

C6—C5—C4	121.4 (3)	O2^{ii}—Cu1—O3	124.25 (7)
C6—C5—H5	119.3	O1^{ii}—Cu1—O3^{ii}	90.02 (10)
C4—C5—H5	119.3	O1—Cu1—O3^{ii}	89.98 (10)
C5—C6—C7	120.8 (3)	O2—Cu1—O3^{ii}	124.25 (7)
C5—C6—H6	119.6	O2^{ii}—Cu1—O3^{ii}	55.75 (7)
C7—C6—H6	119.6	O3—Cu1—O3^{ii}	180.0
N1—C7—C6	120.0 (3)	O1^{ii}—Cu1—C1^{ii}	89.14 (10)
N1—C7—C2	121.8 (2)	O1—Cu1—C1^{ii}	90.86 (10)
C6—C7—C2	118.3 (2)	O2—Cu1—C1^{ii}	152.03 (9)
N1—C8—C9	114.5 (2)	O2^{ii}—Cu1—C1^{ii}	27.97 (9)
N1—C8—H8A	108.6	O3—Cu1—C1^{ii}	152.22 (7)
C9—C8—H8A	108.6	O3^{ii}—Cu1—C1^{ii}	27.78 (7)
N1—C8—H8B	108.6	C7—N1—C8	123.9 (2)
C9—C8—H8B	108.6	C7—N1—H1	114.5
H8A—C8—H8B	107.6	C8—N1—H1	120.0
C10—C9—C11	117.6 (3)	Cu1—O1—H1A	112.8
C10—C9—C8	122.3 (3)	Cu1—O1—H1B	112.1
C11—C9—C8	120.0 (3)	H1A—O1—H1B	108.2
C9—C10—C11^{i}	121.7 (3)	C1—O2—Cu1	104.92 (17)
C9—C10—H10	119.1	C1—O3—Cu1	78.92 (16)
C11^{i}—C10—H10	119.1		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3	0.84	2.00	2.676 (3)	137
O1—H1*A*···O3^{iii}	0.85	2.17	3.011 (3)	174
O1—H1*B*···O4^{ii}	0.85	2.28	3.104 (3)	164
O4—H4*A*···O2^{iv}	0.85	2.03	2.855 (3)	163

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