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catena-Poly[[[diaquadinitratocopper(II)]-μ-4,4′-bipyridine] hemihydrate]

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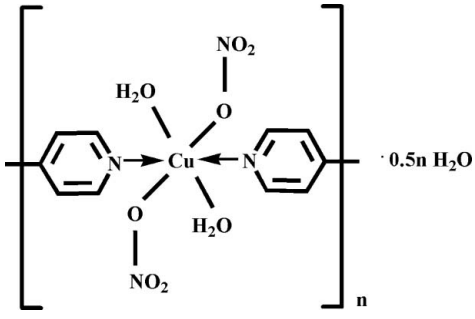
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; H-atom completeness 93%; disorder in solvent or counterion; R factor = 0.049; wR factor = 0.157; data-to-parameter ratio = 16.0.

The title compound, $\{[Cu(C_{10}H_8N_2)(NO_3)_2(H_2O)_2]\cdot 0.5H_2O\}_n$, has a linear polymeric structure, with the bridging ligand 4,4′-bipyridine (bipy) connecting the Cu^{II} ions. Each ion lies on an inversion center and has a distorted octahedral environment, being coordinated by two bipy ligands, two nitrate anions and two water molecules [Cu—N = 2.010 (3) Å and Cu—O = 1.981 (3) and 2.414 (3) Å]. In the crystal structure, the linear polymeric chains, propagating in two directions, are linked by intermolecular O—H···O hydrogen bonds, resulting in a three-dimensional supramolecular network, which has channels parallel to the c axis containing the water molecules of crystallization. The water molecule is equally disordered over two positions.

Related literature

For related literature, see: Ghosh *et al.* (2005); Lu *et al.* (2006); Woodward *et al.* (2006).



Experimental

Crystal data

$[Cu(C_{10}H_8N_2)(NO_3)_2(H_2O)_2]\cdot 0.5H_2O$
M_r = 387.78
Orthorhombic, *Pccn*
a = 12.014 (7) Å
b = 18.533 (8) Å
c = 7.411 (3) Å
V = 1650.1 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.37 mm^{-1}
T = 293 (2) K
0.23 × 0.20 × 0.18 mm

Data collection

Rigaku Weissenberg IP diffractometer
Absorption correction: multi-scan (*TEXRAY*; Molecular Structure Corporation, 1999)
T_{min} = 0.737, T_{max} = 0.803
14611 measured reflections
1892 independent reflections
1281 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
Standard reflections: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.157
S = 1.12
1892 reflections
118 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.981 (3)	Cu1—O2	2.414 (3)
Cu1—N1	2.010 (3)		
O1—Cu1—N1^{i}	90.79 (12)	O1—Cu1—O2	100.91 (10)
O1—Cu1—N1	89.21 (12)	N1^{i}—Cu1—O2	92.33 (10)
O1^{i}—Cu1—O2	79.09 (10)	N1—Cu1—O2	87.67 (10)

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—H01B···O4^{ii}	0.812 (19)	1.94 (2)	2.744 (4)	171 (5)
O1—H01A···O4^{iii}	0.805 (19)	1.94 (2)	2.718 (4)	161 (4)

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

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); 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: CV2233).

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supplementary materials

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catena-Poly[[[diaquadinitratocopper(II)]-μ-4,4'-bipyridine] hemihydrate]

X.-C. Lin, H. Yin and Y. Lin

Comment

Supramolecular architectures based on –*M*-bipy-M– have been receiving increasing attention, which are often extended through weaker interactions including hydrogen bonding and πi-πi stacking (Woodward *et al.*, 2006; Lu *et al.*, 2006; Ghosh *et al.*, 2005). In this work, we chose 4,4'-bipyridine as a spacer ligand to react with a copper salt, resulting in the novel one-dimensional title compound, $\{[Cu(C_{10}H_8N_2)(NO_3)_2(H_2O)_2]\cdot 0.5(H_2O)\}_n$ (I), which are linked into three-dimensional architecture by intermolecular hydrogen bonds.

Part of the chain structure of (I) is shown in Fig. 1. Each Cu (II) center is situated on an inversion center, coordinated by two N atoms of two bridging bipy ligands, two water molecules and two nitrato anions in a distorted octahedral environment. The bipy ligand bridges the adjacent Cu(II) centers, leading to the formation of linear –Cu-bipy-Cu- chains in which the distance of two neighboring Cu(II) centers is 11.043 (4) Å, and the nearest Cu···Cu (x + 1/2, −y + 1, −z − 1/2) interchain separation is 7.058 (3) Å.

In the packing diagram, the linear chains are arranged in a cross-like fashion and linked by numerous intermolecular hydrogen bonds O—H···O between the coordinated water molecules and nitrato anions (Table 2) (Fig. 2), resulting in a three-dimensional supramolecular array. The rhombic channels running along

the *c* axis (Fig. 2) are filled with the disordered crystalline water molecules.

Experimental

An ethanol solution of 4,4'-bipyridine(0.1 mmol) was added to one side of a H-tube, and an ethanol solution of $Cu(NO_3)_2$(0.1 mmol) was added to another side of the H-tube. The tube stood at room temperature for about one and a half month, and well shaped crystals of (I) were obtained.

Refinement

Atom O1W of the crystalline water molecule is disordered between two positions, A and B, respectively. The final occupancy factors for the atoms O1WA and O1WB were assigned to 0.25 each. The H atoms attached to O1WA and O1WB were not positioned. H atoms of the coordinated water molecule were located from difference maps and refined with the O—H distances restrained to 0.82 (1) Å. All other H atoms were positioned geometrically and treated as riding [C—H=0.93Å and U_{iso}(H)=1.2Ueq(C)].

Figures

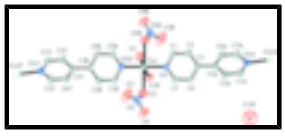

Fig. 1. Part of the polymeric chain structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. All H atoms have been omitted for clarity. [Symmetry codes: (A) −*x* + 1/2, −*y* + 1.5, *z*; (B) −*x*, −*y* + 1, −*z*; (C) *x* − 1/2, *y* − 1/2, −*z*; (D) −*x* − 1/2, −*y* + 1/2, *z*.]

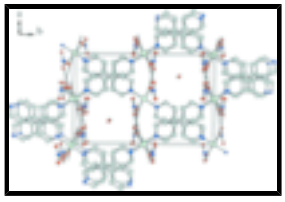

Fig. 2. Packing of (I) viewed down the *c* axis, showing the intermolecular hydrogen bonds as dotted lines. H atoms not-involved in hydrogen bonding have been omitted.

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Crystal data

$[Cu(C_{10}H_8N_2)(NO_3)_2(H_2O)_2]\cdot 0.5H_2O$	F_{000} = 788
M_r = 387.78	D_x = 1.561 Mg m^{-3}
Orthorhombic, *Pccn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ab 2ac	Cell parameters from 9004 reflections
a = 12.014 (7) Å	θ = 3.4–27.6º
b = 18.533 (8) Å	μ = 1.37 mm^{-1}
c = 7.411 (3) Å	*T* = 293 (2) K
V = 1650.1 (14) Å^3	Block, blue
Z = 4	0.23 × 0.20 × 0.18 mm

Data collection

Rigaku Weissenberg IP diffractometer	1892 independent reflections
Radiation source: rotor target	1281 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.054
T = 293(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.4º
Absorption correction: multi-scan (TEXRAY; Molecular Structure Corporation, 1999)	*h* = −15→15
T_{min} = 0.737, T_{max} = 0.803	*k* = −24→24
14611 measured reflections	*l* = −9→9

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.049	H atoms treated by a mixture of independent and constrained refinement

$wR(F^2) = 0.157$	$w = 1/[\sigma^2(F_o^2) + (0.0874P)^2 + 0.4871P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.12$	$(\Delta/\sigma)_{max} < 0.001$
1892 reflections	$\Delta\rho_{max} = 0.87$ e Å^{-3}
118 parameters	$\Delta\rho_{min} = -0.35$ e Å^{-3}
2 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}	Occ. (<1)
Cu1	0.0000	0.5000	0.0000	0.0295 (2)	
O1	−0.1229 (2)	0.54296 (15)	0.1421 (3)	0.0432 (6)	
H01A	−0.126 (4)	0.543 (2)	0.251 (3)	0.056 (12)*	
H01B	−0.184 (2)	0.546 (2)	0.095 (6)	0.064 (14)*	
O2	0.1102 (2)	0.44599 (15)	0.2366 (3)	0.0539 (7)	
O3	−0.0023 (3)	0.4179 (3)	0.4510 (7)	0.0966 (16)	
O4	0.1711 (3)	0.43196 (19)	0.5051 (3)	0.0585 (8)	
N1	0.0885 (2)	0.59087 (14)	0.0366 (4)	0.0336 (6)	
N2	0.0904 (3)	0.43241 (17)	0.3962 (4)	0.0439 (7)	
C1	0.0439 (3)	0.65525 (19)	0.0012 (5)	0.0394 (8)	
H1A	−0.0310	0.6574	−0.0299	0.047*	
C2	0.1038 (3)	0.71886 (17)	0.0087 (5)	0.0402 (8)	
H2A	0.0693	0.7626	−0.0173	0.048*	
C3	0.2153 (3)	0.71715 (15)	0.0551 (5)	0.0323 (7)	
C4	0.2612 (3)	0.64983 (16)	0.0930 (5)	0.0394 (8)	
H4A	0.3359	0.6460	0.1241	0.047*	
C5	0.1958 (3)	0.58901 (17)	0.0842 (5)	0.0394 (8)	
H5A	0.2276	0.5447	0.1126	0.047*	
O1WB	0.7500	0.7500	0.352 (6)	0.190 (16)*	0.25
O1WA	0.7500	0.7500	0.155 (5)	0.162 (13)*	0.25

Atomic displacement parameters (Å^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Cu1	0.0220 (3)	0.0297 (3)	0.0369 (4)	−0.00525 (18)	−0.0001 (2)	−0.0010 (2)
O1	0.0279 (14)	0.0664 (16)	0.0353 (14)	0.0009 (11)	−0.0004 (10)	−0.0099 (13)
O2	0.0491 (17)	0.0749 (18)	0.0377 (13)	0.0021 (13)	−0.0044 (11)	0.0083 (13)
O3	0.042 (2)	0.157 (5)	0.091 (2)	−0.038 (2)	0.0125 (18)	0.002 (3)
O4	0.0395 (16)	0.097 (2)	0.0391 (14)	−0.0062 (15)	−0.0082 (11)	−0.0008 (13)
N1	0.0235 (14)	0.0323 (13)	0.0450 (14)	−0.0042 (11)	−0.0034 (11)	−0.0006 (12)
N2	0.0322 (17)	0.0560 (17)	0.0436 (16)	−0.0112 (13)	0.0000 (13)	0.0010 (14)
C1	0.0242 (17)	0.0363 (17)	0.058 (2)	−0.0018 (14)	−0.0050 (14)	0.0036 (14)
C2	0.0237 (17)	0.0309 (16)	0.066 (2)	0.0008 (12)	−0.0041 (15)	0.0045 (14)
C3	0.0241 (16)	0.0288 (14)	0.0441 (16)	−0.0034 (12)	−0.0008 (13)	0.0003 (13)
C4	0.0246 (16)	0.0333 (14)	0.060 (2)	−0.0012 (13)	−0.0104 (15)	−0.0006 (16)
C5	0.0282 (17)	0.0314 (14)	0.059 (2)	0.0002 (13)	−0.0109 (15)	0.0019 (15)

Geometric parameters (Å, °)

Cu1—O1^{i}	1.981 (3)	N1—C5	1.336 (4)
Cu1—O1	1.981 (3)	C1—C2	1.382 (5)
Cu1—N1^{i}	2.010 (3)	C1—H1A	0.9300
Cu1—N1	2.010 (3)	C2—C3	1.383 (5)
Cu1—O2	2.414 (3)	C2—H2A	0.9300
Cu1—O2^{i}	2.414 (3)	C3—C4	1.393 (4)
O1—H01A	0.805 (19)	C3—C3^{ii}	1.477 (6)
O1—H01B	0.812 (19)	C4—C5	1.376 (4)
O2—N2	1.232 (4)	C4—H4A	0.9300
O3—N2	1.216 (4)	C5—H5A	0.9300
O4—N2	1.261 (4)	O1WB—O1WA	1.46 (6)
N1—C1	1.334 (4)		
O1^{i}—Cu1—O1	180.0	C1—N1—Cu1	120.7 (2)
O1^{i}—Cu1—N1^{i}	89.21 (12)	C5—N1—Cu1	121.6 (2)
O1—Cu1—N1^{i}	90.79 (12)	O3—N2—O2	122.8 (4)
O1^{i}—Cu1—N1	90.79 (12)	O3—N2—O4	119.3 (4)
O1—Cu1—N1	89.21 (12)	O2—N2—O4	117.9 (3)
N1^{i}—Cu1—N1	180.00 (8)	N1—C1—C2	123.1 (3)
O1^{i}—Cu1—O2	79.09 (10)	N1—C1—H1A	118.5
O1—Cu1—O2	100.91 (10)	C2—C1—H1A	118.5
N1^{i}—Cu1—O2	92.33 (10)	C1—C2—C3	119.6 (3)
N1—Cu1—O2	87.67 (10)	C1—C2—H2A	120.2
O1^{i}—Cu1—O2^{i}	100.91 (10)	C3—C2—H2A	120.2
O1—Cu1—O2^{i}	79.09 (10)	C2—C3—C4	117.0 (3)
N1^{i}—Cu1—O2^{i}	87.67 (10)	C2—C3—C3^{ii}	121.9 (3)
N1—Cu1—O2^{i}	92.33 (10)	C4—C3—C3^{ii}	121.0 (4)
O2—Cu1—O2^{i}	180.0	C5—C4—C3	119.9 (3)
Cu1—O1—H01A	125 (3)	C5—C4—H4A	120.1
Cu1—O1—H01B	118 (3)	C3—C4—H4A	120.1
H01A—O1—H01B	113 (5)	N1—C5—C4	122.8 (3)
N2—O2—Cu1	132.5 (2)	N1—C5—H5A	118.6

C1—N1—C5	117.5 (3)	C4—C5—H5A	118.6
O1^{i}—Cu1—O2—N2	−165.3 (3)	O2^{i}—Cu1—N1—C5	−146.5 (3)
O1—Cu1—O2—N2	14.7 (3)	Cu1—O2—N2—O3	30.3 (6)
N1^{i}—Cu1—O2—N2	−76.6 (3)	Cu1—O2—N2—O4	−151.6 (3)
N1—Cu1—O2—N2	103.4 (3)	C5—N1—C1—C2	1.1 (5)
O2^{i}—Cu1—O2—N2	113 (74)	Cu1—N1—C1—C2	−174.1 (3)
O1^{i}—Cu1—N1—C1	129.5 (3)	N1—C1—C2—C3	−0.1 (5)
O1—Cu1—N1—C1	−50.5 (3)	C1—C2—C3—C4	−0.3 (5)
N1^{i}—Cu1—N1—C1	43.7 (6)	C1—C2—C3—C3^{ii}	176.4 (3)
O2—Cu1—N1—C1	−151.4 (3)	C2—C3—C4—C5	−0.3 (5)
O2^{i}—Cu1—N1—C1	28.6 (3)	C3^{ii}—C3—C4—C5	−177.1 (3)
O1^{i}—Cu1—N1—C5	−45.6 (3)	C1—N1—C5—C4	−1.8 (5)
O1—Cu1—N1—C5	134.4 (3)	Cu1—N1—C5—C4	173.5 (3)
N1^{i}—Cu1—N1—C5	−131.4 (3)	C3—C4—C5—N1	1.4 (6)
O2—Cu1—N1—C5	33.5 (3)		

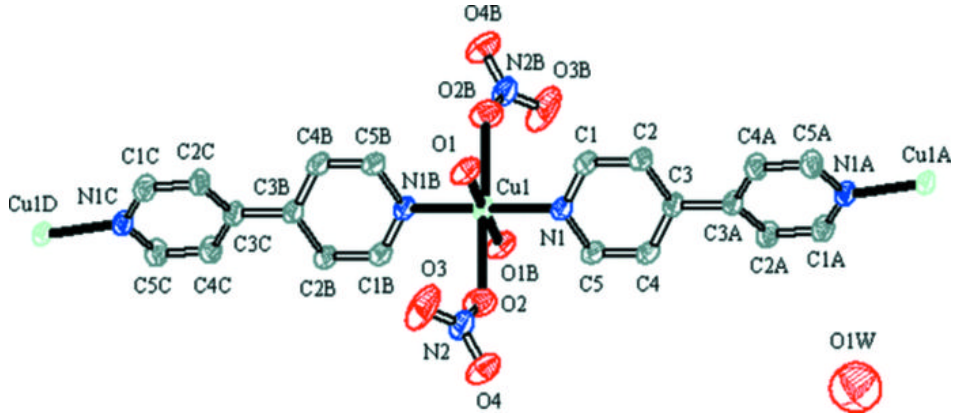
Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) −*x*+1/2, −*y*+3/2, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H01B···O4^{iii}	0.812 (19)	1.94 (2)	2.744 (4)	171 (5)
O1—H01A···O4^{iv}	0.805 (19)	1.94 (2)	2.718 (4)	161 (4)

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

Fig. 1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O3B
O2B
O1
C1
C2
C4A
C5A
N1A
Cu1A
C1C
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C5B
C3
Cu1D
N1C
C3B
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Cu1
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C4
C5C
C4C
C2B
C1B
O2
N2
O1W
O4

Fig. 2