Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[diaquacopper(II)]-μ-hydroxido-κ^2O:O-μ-[4-(4H-1,2,4-triazol-4-yl)benzoato]-κ^2N^1:N^2]

Haochen Shi,[a,b]* Feng Gao[b] and Jingang Qi[b]

[a]College of Physics, Jilin University, Changchun 130012, People's Republic of China, and [b]Department of Physics Education, Changchun Normal University, Changchun 130032, People's Republic of China
Correspondence e-mail: chemshihc@163.com

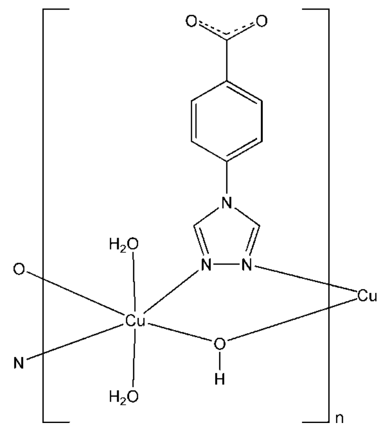
Received 7 August 2011; accepted 11 August 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.028; wR factor = 0.083; data-to-parameter ratio = 10.5.

The title compound, $[Cu(C_9H_6N_3O_2)(OH)(H_2O)_2]_n$, adopts a chain motif along [010] in which the Cu^{II} atoms are bridged by hydroxy groups and 4-(1,2,4-triazol-4-yl)benzoate (tab) ligands. The Cu^{II} atom lies on an inversion center and is six-coordinated by two N atoms from two tab ligands, two hydroxy groups and two water molecules, giving a distorted octahedral geometry. The hydroxy group and the tab ligand are located on a mirror plane. One of the water H atoms is disordered over two positions with equal occupancy factors. Intermolecular O—H⋯O hydrogen bonds extend the chains into a layer parallel to (100) and C—H⋯O hydrogen bonds connect the layers into a three-dimensional network.

Related literature

For general background to the applications of coordination polymers, see: Aghabozorg *et al.* (2008); Liu *et al.* (2010); Wang *et al.* (2009); Zhang *et al.* (2004). For a related structure, see: Lin *et al.* (2011).



Experimental

Crystal data

$[Cu(C_9H_6N_3O_2)(OH)(H_2O)_2]$
M_r = 304.75
Monoclinic, $P2_1/m$
a = 6.787 (5) Å
b = 6.758 (5) Å
c = 12.036 (5) Å
β = 102.919 (5)°
V = 538.1 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.05 mm^{-1}
T = 293 K
0.21 × 0.19 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.64, T_{max} = 0.75
3021 measured reflections
1165 independent reflections
1010 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.083
S = 1.12
1165 reflections
111 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O3—H9⋯O2^{i}	0.84 (3)	2.07 (3)	2.907 (4)	172 (3)
O4—H10A⋯O2^{ii}	0.83 (3)	1.94 (3)	2.746 (3)	164 (3)
O4—H10⋯O4^{iii}	0.85 (6)	1.94 (6)	2.762 (4)	165 (6)
O4—H10′⋯O4^{iv}	0.85 (2)	1.93 (2)	2.759 (4)	165 (7)
C6—H6⋯O1^{v}	0.93	2.44	3.172 (5)	135
C8—H8⋯O1^{vi}	0.93	2.23	3.052 (4)	147

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank Jilin University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2457).

References

Aghabozorg, H., Manteghi, F. & Sheshmani, S. (2008). *J. Iran. Chem. Soc.* **5**, 184–227.
Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Lin, M.-H., Zhou, J.-F., Liu, B.-B. & Lin, J.-L. (2011). *Acta Cryst.* E**67**, m352.
Liu, D., Ren, Z.-G., Li, H.-X., Chen, Y., Wang, J., Zhang, Y. & Lang, J.-P. (2010). *CrystEngComm*, **12**, 1912–1919.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, G.-H., Li, Z.-G., Jia, H.-Q., Hu, N.-H. & Xu, J.-W. (2009). *Acta Cryst.* E**65**, m1568–m1569.
Zhang, J., Li, Z.-J., Kang, Y., Cheng, J.-K. & Yao, Y.-G. (2004). *Inorg. Chem.* **43**, 8085–8091.

supporting information

Acta Cryst. (2011). E**67**, m1255–m1256 [doi:10.1107/S1600536811032624]

catena-Poly[[diaquacopper(II)]-μ-hydroxido-κ^2O:O-μ-[4-(4*H*-1,2,4-triazol-4-yl)benzoato]-κ^2N^1:N^2]

Haochen Shi, Feng Gao and Jingang Qi

S1. Comment

Coordination polymers are currently of great interest due to structural versatility, unique properties and potential applications in catalysis, gas storage and in molecular-based magnetic materials (Liu *et al.*, 2010; Zhang *et al.*, 2004). Heterocyclic carboxylates have often been used as mono-, bi- or multidentate ligands to bind transition metal centers, leading to the formation of moderately robust metal–organic coordination frameworks (Aghabozorg *et al.*, 2008; Wang *et al.*, 2009). In this contribution, we selected 4-(1,2,4-triazol-4-yl)benzoic acid (Htab) as an organic carboxylate ligand, generating a coordination polymer, $[Cu(C_9H_6N_3O_2)(H_2O)_2(OH)]$, which is reported here.

The title compound adopts a chain motif, in which the hydroxy groups and tab ligands as bridges to connect adjacent octahedrally coordinated Cu^{II} atoms (Fig. 1). The Cu^{II} atom lies on an inversion center and is six-coordinated by two N atoms from two tab ligands, two O atoms from hydroxy groups and two water molecules, giving a distorted octahedral geometry. The Cu—O and Cu—N bond lengths and the O—Cu—O, O—Cu—N and N—Cu—N bond angles are in the normal range (Lin *et al.*, 2011). The hydroxy group and the tab ligand are located on a mirro plane. One of the water H atoms is disordered over two positions with equal occupancy factors. Intermolecular O—H···O hydrogen bonds extend the chains into a layer parallel to (1 0 0). C—H···O hydrogen bonds connect the layers into a three-dimensional network (Fig. 2).

S2. Experimental

The synthesis was performed under hydrothermal conditions. A mixture of $CuCl_2.2H_2O$ (0.2 mmol, 0.034 g), 4-(1,2,4-triazol-4-yl)benzoic acid (0.2 mmol, 0.038 g), NaOH (0.2 mmol, 0.008 g) and H_2O (15 ml) in a 25 ml stainless steel reactor with a Teflon liner was heated from 293 to 433 K and a constant temperature was maintained at 433 K for 96 h. After the mixture was cooled to 293 K, blue crystals of the title compound were obtained from the reaction.

S3. Refinement

H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). H atoms bonded to O atoms were located in a difference Fourier map and refined with O—H distance restraints of 0.85 (1) Å and with U_{iso}(H) = 1.5U_{eq}(O).

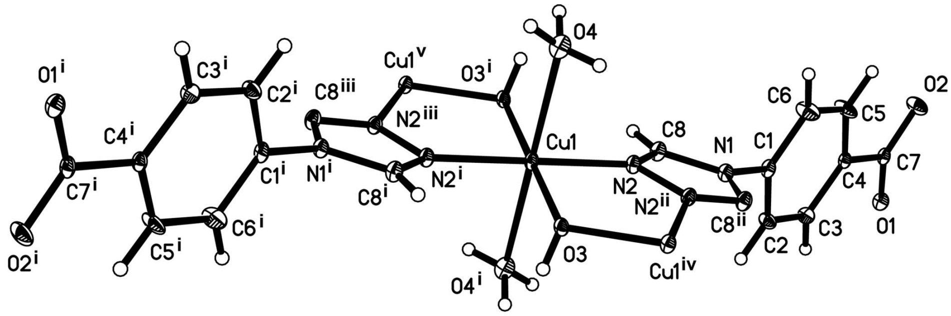


Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. One H atom of water molecule (O4) is disordered over two positions with equal occupancy factors. [Symmetry codes: (i) *-x*, *-y*, *-z*; (ii) *x*, 1/2 - *y*, *z*; (iii) *-x*, *y* - 1/2, *-z*; (iv) *x*, *y* - 1/2, *z*; (v) *x*, *y* + 1/2, *z*.]

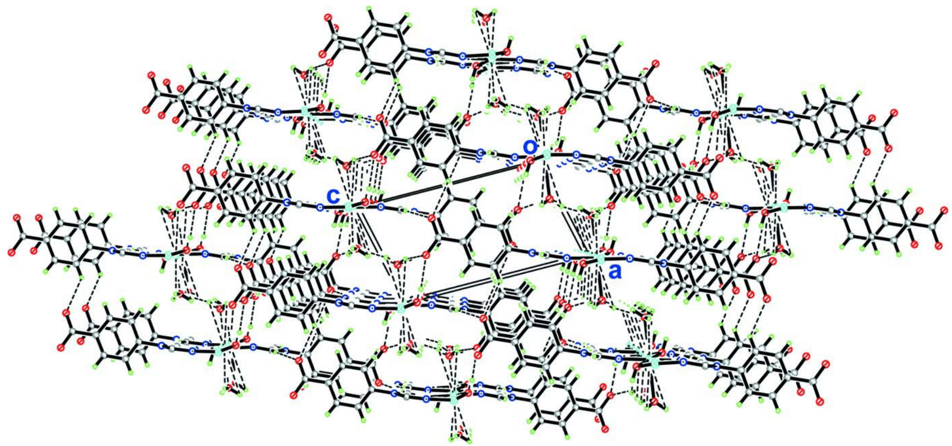


Figure 2

View of the three-dimensional structure of the title compound, built by hydrogen bonds (dashed lines).

catena-Poly[[diaquacopper(II)]-*μ*-hydroxido-κ^2O:*O*- *μ*-[4-(4*H*-1,2,4-triazol-4-yl)benzoato]- κ^2N^1:N^2]

Crystal data

$[Cu(C_9H_6N_3O_2)(OH)(H_2O)_2]$
M_r = 304.75
Monoclinic, $P2_1/m$
Hall symbol: -P 2yb
a = 6.787 (5) Å
b = 6.758 (5) Å
c = 12.036 (5) Å
β = 102.919 (5)°
V = 538.1 (6) Å^3
Z = 2
F(000) = 310
D_x = 1.881 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 1165 reflections
θ = 1.0–26.1°
μ = 2.05 mm^{-1}
T = 293 K
Block, blue
0.21 × 0.19 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.64, T_{max} = 0.75
3021 measured reflections
1165 independent reflections

1010 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 26.1°$, $\theta_{min} = 3.1°$
$h = -7 \rightarrow 8$
$k = -7 \rightarrow 8$
$l = -14 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.083$
$S = 1.12$
1165 reflections
111 parameters
4 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
$w = 1/[\sigma^2(F_o^2) + (0.0403P)^2 + 0.5502P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.2717 (6)	0.2500	−0.3753 (3)	0.0147 (7)	
C2	0.4779 (6)	0.2500	−0.3610 (3)	0.0185 (8)	
H2	0.5611	0.2500	−0.2882	0.022*	
C3	0.5609 (6)	0.2500	−0.4564 (3)	0.0176 (8)	
H3	0.7006	0.2500	−0.4473	0.021*	
C4	0.4374 (5)	0.2500	−0.5653 (3)	0.0135 (7)	
C5	0.2310 (6)	0.2500	−0.5770 (3)	0.0264 (10)	
H5	0.1474	0.2500	−0.6496	0.032*	
C6	0.1448 (6)	0.2500	−0.4827 (3)	0.0279 (10)	
H6	0.0052	0.2500	−0.4915	0.033*	
C7	0.5284 (6)	0.2500	−0.6686 (3)	0.0148 (7)	
C8	0.1359 (4)	0.0900 (4)	−0.2195 (2)	0.0174 (6)	
H8	0.1530	−0.0410	−0.2390	0.021*	
N1	0.1836 (5)	0.2500	−0.2760 (2)	0.0151 (7)	
N2	0.0624 (3)	0.1479 (3)	−0.13349 (17)	0.0150 (5)	
O1	0.7151 (4)	0.2500	−0.6538 (2)	0.0184 (6)	
O2	0.4060 (4)	0.2500	−0.7656 (2)	0.0260 (7)	
Cu1	0.0000	0.0000	0.0000	0.01409 (17)	
O3	0.0096 (4)	0.2500	0.0802 (2)	0.0145 (5)	
O4	−0.3805 (3)	0.0459 (3)	−0.07541 (19)	0.0254 (5)	
H9	0.118 (4)	0.2500	0.130 (3)	0.038*	
H10A	−0.413 (5)	−0.040 (4)	−0.126 (2)	0.038*	
H10	−0.471 (8)	0.017 (11)	−0.040 (6)	0.038*	0.50
H10′	−0.372 (10)	0.169 (2)	−0.086 (6)	0.038*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0200 (19)	0.0156 (18)	0.0121 (18)	0.000	0.0112 (15)	0.000
C2	0.0175 (19)	0.026 (2)	0.0116 (18)	0.000	0.0030 (15)	0.000

C3	0.0141 (18)	0.023 (2)	0.0166 (18)	0.000	0.0064 (15)	0.000
C4	0.0189 (18)	0.0116 (17)	0.0118 (18)	0.000	0.0071 (15)	0.000
C5	0.019 (2)	0.053 (3)	0.0076 (18)	0.000	0.0021 (15)	0.000
C6	0.0142 (19)	0.051 (3)	0.020 (2)	0.000	0.0059 (16)	0.000
C7	0.0224 (19)	0.0125 (18)	0.0121 (18)	0.000	0.0092 (15)	0.000
C8	0.0221 (13)	0.0154 (13)	0.0172 (13)	0.0008 (11)	0.0096 (11)	−0.0004 (11)
N1	0.0174 (16)	0.0186 (16)	0.0121 (15)	0.000	0.0090 (12)	0.000
N2	0.0193 (11)	0.0134 (11)	0.0140 (10)	0.0011 (9)	0.0073 (9)	0.0003 (9)
O1	0.0196 (14)	0.0210 (14)	0.0178 (14)	0.000	0.0110 (11)	0.000
O2	0.0230 (15)	0.0456 (19)	0.0098 (13)	0.000	0.0046 (11)	0.000
Cu1	0.0197 (3)	0.0131 (3)	0.0117 (2)	0.00017 (17)	0.00825 (18)	0.00091 (17)
O3	0.0205 (14)	0.0146 (13)	0.0095 (12)	0.000	0.0056 (10)	0.000
O4	0.0300 (11)	0.0221 (11)	0.0270 (11)	−0.0001 (10)	0.0124 (9)	−0.0014 (9)

Geometric parameters (Å, º)

C1—C2	1.371 (5)	C7—O2	1.272 (4)
C1—C6	1.383 (5)	C8—N2	1.306 (3)
C1—N1	1.452 (4)	C8—N1	1.354 (3)
C2—C3	1.388 (5)	C8—H8	0.9300
C2—H2	0.9300	N2—N2^{i}	1.381 (4)
C3—C4	1.389 (5)	Cu1—O3	1.9397 (16)
C3—H3	0.9300	Cu1—N2^{ii}	2.016 (2)
C4—C5	1.376 (6)	Cu1—O4	2.558 (3)
C4—C7	1.508 (5)	O3—H9	0.839 (10)
C5—C6	1.388 (5)	O4—H10A	0.836 (10)
C5—H5	0.9300	O4—H10	0.846 (10)
C6—H6	0.9300	O4—H10′	0.844 (10)
C7—O1	1.239 (5)		
C2—C1—C6	121.5 (3)	N2—C8—N1	109.6 (2)
C2—C1—N1	119.5 (3)	N2—C8—H8	125.2
C6—C1—N1	119.0 (3)	N1—C8—H8	125.2
C1—C2—C3	119.2 (3)	C8—N1—C8^{i}	105.9 (3)
C1—C2—H2	120.4	C8—N1—C1	127.03 (15)
C3—C2—H2	120.4	C8^{i}—N1—C1	127.03 (15)
C2—C3—C4	120.6 (3)	C8—N2—N2^{i}	107.42 (16)
C2—C3—H3	119.7	C8—N2—Cu1	132.01 (19)
C4—C3—H3	119.7	N2^{i}—N2—Cu1	119.72 (6)
C5—C4—C3	118.9 (3)	O3—Cu1—N2	88.58 (10)
C5—C4—C7	120.7 (3)	O3—Cu1—N2^{ii}	91.42 (10)
C3—C4—C7	120.4 (3)	N2—Cu1—N2^{ii}	180.00 (11)
C4—C5—C6	121.4 (4)	O3—Cu1—O4	89.42 (9)
C4—C5—H5	119.3	O3—Cu1—O4^{ii}	90.58 (9)
C6—C5—H5	119.3	N2—Cu1—O4^{ii}	88.14 (8)
C1—C6—C5	118.4 (4)	O4—Cu1—N2	91.86 (8)
C1—C6—H6	120.8	Cu1—O3—Cu1^{iii}	121.15 (13)
C5—C6—H6	120.8	Cu1—O3—H9	106.6 (15)

O1—C7—O2	124.7 (3)	H10A—O4—H10	96 (5)
O1—C7—C4	118.4 (3)	H10A—O4—H10′	126 (5)
O2—C7—C4	116.9 (3)	H10—O4—H10′	113 (7)
N2—C8—N1—C8^{i}	0.2 (4)	N1—C8—N2—Cu1	−169.2 (2)
N2—C8—N1—C1	179.1 (3)	C8—N2—Cu1—O3^{ii}	−20.5 (3)
C2—C1—N1—C8	−89.3 (3)	N2^{i}—N2—Cu1—O3^{ii}	171.53 (8)
C6—C1—N1—C8	90.7 (3)	C8—N2—Cu1—O3	159.5 (3)
C2—C1—N1—C8^{i}	89.3 (3)	N2^{i}—N2—Cu1—O3	−8.47 (8)
C6—C1—N1—C8^{i}	−90.7 (3)	N2—Cu1—O3—Cu1^{iii}	15.10 (15)
N1—C8—N2—N2^{i}	−0.2 (2)	N2^{ii}—Cu1—O3—Cu1^{iii}	−164.90 (15)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H9···O2^{iv}	0.84 (3)	2.07 (3)	2.907 (4)	172 (3)
O4—H10*A*···O2^{v}	0.83 (3)	1.94 (3)	2.746 (3)	164 (3)
O4—H10···O4^{vi}	0.85 (6)	1.94 (6)	2.762 (4)	165 (6)
O4—H10′···O4^{i}	0.85 (2)	1.93 (2)	2.759 (4)	165 (7)
C6—H6···O1^{vii}	0.93	2.44	3.172 (5)	135
C8—H8···O1^{viii}	0.93	2.23	3.052 (4)	147

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