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catena-Poly[[[bis(benzoato-κO)-copper(II)]-μ-1,1′-(3-oxapentane-1,5-diyl)diimidazole] monohydrate]

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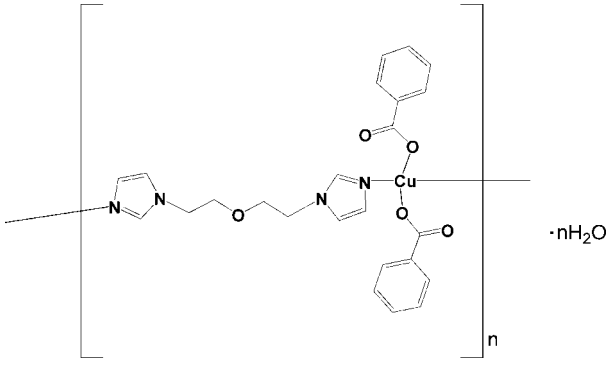
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.046; wR factor = 0.123; data-to-parameter ratio = 14.7.

In the title compound, $\{[Cu(C_7H_5O_2)_2(C_{10}H_{14}N_4O)]\cdot H_2O\}_n$ or $\{[Cu(BA)_2(BIE)]\cdot H_2O\}_n$, where BA is the benzoate anion and BIE is 2,2′-bis(imidazolethyl), the Cu^{II} atom, which lies on an inversion centre, is coordinated in a square-planar geometry by two N atoms from two BIE ligands and two O atoms from two benzoate anions. The ether and water O atoms are located on twofold axes. The Cu^{II} atoms are linked *via* BIE ligands to form a one-dimensional chain structure along the c axis. The chains are further connected through hydrogen-bonding interactions between the water molecules and the carboxylate O atoms of the BA anions, resulting in a two-dimensional supramolecular network. The C atom and H atoms of the ethyl chain are disordered over two positions with refined occupancies of 0.583 (12) and 0.417 (12).

Related literature

For related literature, see: Yang *et al.* (2007); Yang, Ma *et al.* (2006); Yang, Yue *et al.* (2006).



Experimental

Crystal data

$[Cu(C_7H_5O_2)_2(C_{10}H_{14}N_4O)]\cdot H_2O$
M_r = 530.04
Monoclinic, $P2/n$
a = 11.4960 (15) Å
b = 7.7400 (16) Å
c = 13.609 (3) Å
β = 103.140 (3)°
V = 1179.2 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.97 mm^{-1}
T = 293 (2) K
0.11 × 0.11 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.901, T_{max} = 0.907
10769 measured reflections
2697 independent reflections
1980 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.123
S = 1.10
2697 reflections
183 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1A···O1^{i}	0.85 (4)	2.08 (5)	2.862 (3)	153 (4)

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); 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: RZ2175).

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supplementary materials

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catena-Poly[[[bis(benzoato-*κO*)copper(II)]-*μ*-1,1'-(3-oxapentane-1,5-diyl)diimidazole] monohydrate]

G.-H. Wei, J. Liu, H.-Y. Bai and J. Yang

Comment

The design and synthesis of coordination polymers has received much attention due to their interesting structures and potential applications in ion exchange and gas storage (Yang, Yue *et al.*, 2006). In this regard, chain structures are particularly interesting (Yang *et al.*, 2007). We selected 2,2'-bis(imidazol)ether (BIE) as a bridging ligand, generating a new chain coordination polymer, $\{[Cu(BA)_2(BIE)]\cdot H_2O\}_n$, whose structure is reported here.

In the title compound, the copper(II) atom, which lies on an inversion centre, displays a square-planar coordination geometry provided by two nitrogen atoms from two BIE ligands and two oxygen atoms from two distinct benzoate anions (Fig. 1). The Cu—O and Cu—N distances (Cu1—N1 = 1.985 (2) Å, Cu1–O2 = 1.968 (2) Å) are within their normal ranges (Yang, Ma *et al.*, 2006). The copper(II) centers are linked *via* BIE ligands to form a one-dimensional chain structure along the *c* axis (Fig. 2). The monodentate BA anions are located on both sides of the chain. The adjacent chains are further connected through hydrogen bonds between BA anions and water molecules (Table 2), thus forming a two-dimensional supramolecular network (Fig. 3). The ether (O3) and water (O1W) oxygen atoms lie on twofold axes. The C11, C12 carbon atom and attached H atoms are disordered over two positions with refined occupancies of 0.583 (12) and 0.417 (12).

Experimental

A mixture of $CuCl_2\cdot 2H_2O$ (86.0 mg, 0.5 mmol) and NaOH (40 mg, 1 mmol) in 20 ml water was stirred for 10 min at room temperature, then the $Cu(OH)_2$ precipitate was filtered. HBA (122.0 mg, 1 mmol) was added to the $Cu(OH)_2$ suspension in C_2H_5OH/H_2O (1:4 *v*/*v*) with constant stirring for 1 h until a blue precipitate was obtained. The solid was filtered off and washed with water, then BIE (103.1 mg, 0.5 mmol) was added with stirring for 1 h to give a blue solution. Blue crystals of the title compound were obtained on slow evaporation of the solvent at room temperature.

Refinement

All H atoms bound to C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93–0.97 Å and U_{iso} = 1.2U_{eq}(C). The independent water H atom was located in a difference Fourier map and refined with U_{iso}(H) = 1.5U_{eq}(O) and with the O—H distance constrained to 0.85 Å.

Figures

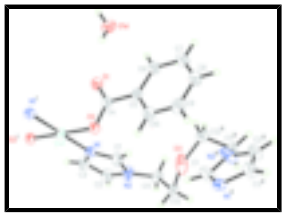

Fig. 1. *ORTEP* view of title compound showing 50% probability ellipsoids. Symmetry code: (i) −*x*, −*y*, −*z* + 1; (ii) −*x* + 1/2, *y*, −*z* + 3/2.

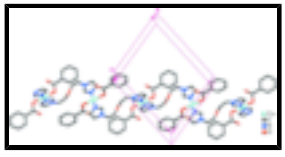

Fig. 2. View of the one-dimensional polymeric chain of the title compound. H atoms are omitted for clarity.

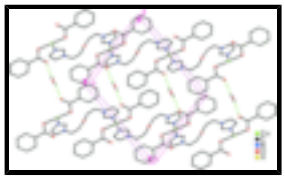

Fig. 3. View of the two-dimensional supramolecular network *via* hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding are omitted for clarity.

catena-Poly[[[bis(benzoato-κ*O*)copper(II)]-μ-1,1'- (3-oxapentane-1,5-diyl)diimidazole] monohydrate]

Crystal data

$[Cu(C_7H_5O_2)_2(C_{10}H_{14}N_4O)]\cdot H_2O$	F_{000} = 550
M_r = 530.04	D_x = 1.493 Mg m^{-3}
Monoclinic, *P*2/*n*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2yac	Cell parameters from 7716 reflections
a = 11.4960 (15) Å	θ = 3.0–27.5º
b = 7.7400 (16) Å	μ = 0.97 mm^{-1}
c = 13.609 (3) Å	*T* = 293 (2) K
β = 103.140 (3)º	Block, blue
V = 1179.2 (4) Å^3	0.11 × 0.11 × 0.10 mm
Z = 2	

Data collection

Rigaku RAXIS-RAPID diffractometer	2697 independent reflections
Radiation source: rotor target	1980 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.054
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.1º
φ and ω scans	*h* = −14→12
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*k* = −10→10
T_{min} = 0.901, T_{max} = 0.907	*l* = −17→17

10769 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
$R[F^2 > 2\sigma(F^2)] = 0.046$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.123$	$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 0.8067P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} < 0.001$
2697 reflections	$\Delta\rho_{max} = 0.44$ e Å^{-3}
183 parameters	$\Delta\rho_{min} = -0.51$ e Å^{-3}
1 restraint	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	0.0000	0.5000	0.03667 (17)	
C1	0.0488 (3)	−0.3199 (5)	0.6225 (3)	0.0655 (10)	
H1	0.1290	−0.2915	0.6450	0.079*	
C2	−0.1193 (3)	−0.4557 (5)	0.6050 (3)	0.0616 (10)	
H2	−0.1777	−0.5356	0.6112	0.074*	
C3	−0.1333 (3)	−0.3151 (5)	0.5459 (3)	0.0590 (9)	
H3	−0.2051	−0.2808	0.5038	0.071*	
C4	0.2271 (2)	−0.0881 (4)	0.5132 (2)	0.0400 (6)	
C5	0.3558 (2)	−0.1290 (4)	0.5583 (2)	0.0403 (6)	
C6	0.4217 (3)	−0.2260 (5)	0.5036 (2)	0.0508 (8)	
H6	0.3858	−0.2661	0.4394	0.061*	
C7	0.5408 (3)	−0.2624 (6)	0.5451 (3)	0.0649 (10)	
H7	0.5844	−0.3279	0.5087	0.078*	
C8	0.5948 (3)	−0.2028 (6)	0.6391 (3)	0.0669 (10)	
H8	0.6750	−0.2266	0.6660	0.080*	

C9	0.5303 (3)	−0.1074 (5)	0.6939 (3)	0.0620 (10)	
H9	0.5670	−0.0660	0.7575	0.074*	
C10	0.4102 (3)	−0.0734 (5)	0.6537 (2)	0.0501 (8)	
H10	0.3662	−0.0123	0.6917	0.060*	
C11	0.0454 (8)	−0.6286 (12)	0.6974 (8)	0.050 (3)	0.417 (12)
H11A	−0.0168	−0.6987	0.7149	0.060*	0.417 (12)
H11B	0.0824	−0.6922	0.6512	0.060*	0.417 (12)
C12	0.1351 (9)	−0.5730 (14)	0.7888 (8)	0.052 (3)	0.417 (12)
H12A	0.1543	−0.6674	0.8366	0.062*	0.417 (12)
H12B	0.1049	−0.4769	0.8214	0.062*	0.417 (12)
C11'	0.0548 (7)	−0.5492 (11)	0.7543 (7)	0.060 (2)	0.583 (12)
H11C	0.0745	−0.4648	0.8082	0.072*	0.583 (12)
H11D	−0.0016	−0.6309	0.7713	0.072*	0.583 (12)
C12'	0.1665 (7)	−0.6430 (10)	0.7439 (7)	0.067 (2)	0.583 (12)
H12C	0.1908	−0.7266	0.7978	0.081*	0.583 (12)
H12D	0.1538	−0.7025	0.6796	0.081*	0.583 (12)
N1	−0.0276 (2)	−0.2293 (3)	0.55599 (18)	0.0416 (6)	
N2	−0.0022 (3)	−0.4574 (4)	0.6540 (3)	0.0697 (10)	
O1	0.18108 (18)	−0.1261 (3)	0.42329 (15)	0.0494 (5)	
O2	0.16920 (18)	−0.0139 (3)	0.57095 (15)	0.0431 (5)	
O3	0.2500	−0.5163 (5)	0.7500	0.0835 (14)	
O1W	0.2500	−0.2648 (5)	0.2500	0.0689 (10)	
H1A	0.263 (5)	−0.193 (4)	0.207 (3)	0.103*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0352 (3)	0.0402 (3)	0.0364 (3)	0.0039 (2)	0.0117 (2)	0.0030 (2)
C1	0.0405 (17)	0.071 (2)	0.087 (3)	0.0054 (17)	0.0194 (17)	0.038 (2)
C2	0.054 (2)	0.052 (2)	0.079 (3)	−0.0057 (16)	0.0169 (19)	0.0142 (18)
C3	0.0481 (18)	0.057 (2)	0.067 (2)	−0.0066 (16)	0.0034 (16)	0.0101 (18)
C4	0.0366 (14)	0.0382 (16)	0.0452 (16)	−0.0012 (12)	0.0097 (13)	0.0063 (13)
C5	0.0372 (14)	0.0417 (16)	0.0419 (15)	0.0005 (13)	0.0086 (12)	0.0078 (13)
C6	0.0413 (16)	0.063 (2)	0.0479 (17)	0.0043 (15)	0.0099 (13)	−0.0028 (16)
C7	0.0435 (17)	0.089 (3)	0.065 (2)	0.0157 (19)	0.0173 (17)	0.001 (2)
C8	0.0405 (17)	0.097 (3)	0.060 (2)	0.0116 (19)	0.0038 (16)	0.006 (2)
C9	0.0521 (19)	0.078 (3)	0.0486 (18)	−0.0012 (19)	−0.0027 (16)	−0.0014 (18)
C10	0.0482 (17)	0.0537 (19)	0.0476 (17)	0.0018 (15)	0.0094 (14)	−0.0010 (15)
C11	0.058 (5)	0.043 (5)	0.045 (5)	−0.009 (4)	0.004 (4)	0.002 (4)
C12	0.062 (6)	0.046 (5)	0.044 (5)	0.003 (5)	0.007 (5)	0.011 (4)
C11'	0.063 (4)	0.061 (5)	0.054 (5)	−0.002 (4)	0.007 (4)	0.023 (4)
C12'	0.077 (5)	0.047 (4)	0.067 (5)	0.013 (4)	−0.007 (4)	−0.005 (4)
N1	0.0395 (12)	0.0442 (14)	0.0434 (13)	0.0037 (11)	0.0144 (11)	0.0043 (11)
N2	0.0497 (16)	0.0665 (19)	0.098 (2)	0.0122 (15)	0.0279 (17)	0.0449 (18)
O1	0.0429 (11)	0.0594 (14)	0.0441 (11)	0.0040 (10)	0.0060 (9)	−0.0014 (10)
O2	0.0371 (10)	0.0495 (12)	0.0434 (11)	0.0060 (9)	0.0104 (9)	0.0045 (9)
O3	0.053 (2)	0.058 (2)	0.121 (4)	0.000	−0.019 (2)	0.000
O1W	0.095 (3)	0.063 (2)	0.053 (2)	0.000	0.026 (2)	0.000

Geometric parameters (Å, °)

Cu1—O2	1.968 (2)	C8—H8	0.9300
Cu1—O2^{i}	1.968 (2)	C9—C10	1.389 (4)
Cu1—N1	1.985 (2)	C9—H9	0.9300
Cu1—N1^{i}	1.985 (2)	C10—H10	0.9300
C1—N1	1.311 (4)	C11—C12	1.487 (16)
C1—N2	1.333 (4)	C11—N2	1.502 (9)
C1—H1	0.9300	C11—H11A	0.9700
C2—C3	1.341 (5)	C11—H11B	0.9700
C2—N2	1.360 (5)	C12—O3	1.591 (10)
C2—H2	0.9300	C12—H12A	0.9700
C3—N1	1.364 (4)	C12—H12B	0.9700
C3—H3	0.9300	C11'—C12'	1.509 (14)
C4—O1	1.252 (3)	C11'—N2	1.546 (8)
C4—O2	1.276 (3)	C11'—H11C	0.9700
C4—C5	1.501 (4)	C11'—H11D	0.9700
C5—C10	1.376 (4)	C12'—O3	1.362 (8)
C5—C6	1.396 (4)	C12'—H12C	0.9700
C6—C7	1.386 (4)	C12'—H12D	0.9700
C6—H6	0.9300	O3—C12'^{ii}	1.362 (8)
C7—C8	1.369 (5)	O3—C12^{ii}	1.591 (10)
C7—H7	0.9300	O1W—H1A	0.85 (4)
C8—C9	1.380 (5)		
O2—Cu1—O2^{i}	180.0	C12—C11—H11B	111.5
O2—Cu1—N1	89.37 (9)	N2—C11—H11B	111.5
O2^{i}—Cu1—N1	90.63 (9)	H11A—C11—H11B	109.3
O2—Cu1—N1^{i}	90.63 (9)	C11—C12—O3	105.8 (8)
O2^{i}—Cu1—N1^{i}	89.37 (9)	C11—C12—H12A	110.6
N1—Cu1—N1^{i}	180.0	O3—C12—H12A	110.6
N1—C1—N2	112.0 (3)	C11—C12—H12B	110.6
N1—C1—H1	124.0	O3—C12—H12B	110.6
N2—C1—H1	124.0	H12A—C12—H12B	108.7
C3—C2—N2	105.8 (3)	C12'—C11'—N2	109.7 (7)
C3—C2—H2	127.1	C12'—C11'—H11C	109.7
N2—C2—H2	127.1	N2—C11'—H11C	109.7
C2—C3—N1	110.6 (3)	C12'—C11'—H11D	109.7
C2—C3—H3	124.7	N2—C11'—H11D	109.7
N1—C3—H3	124.7	H11C—C11'—H11D	108.2
O1—C4—O2	122.9 (3)	O3—C12'—C11'	104.5 (7)
O1—C4—C5	120.6 (3)	O3—C12'—C12'^{ii}	46.1 (4)
O2—C4—C5	116.5 (3)	C11'—C12'—C12'^{ii}	149.4 (6)
C10—C5—C6	119.1 (3)	O3—C12'—H12C	110.9
C10—C5—C4	121.0 (3)	C11'—C12'—H12C	110.9
C6—C5—C4	120.0 (3)	C12'^{ii}—C12'—H12C	79.7

C7—C6—C5	119.8 (3)	O3—C12'—H12D	110.9
C7—C6—H6	120.1	C11'—C12'—H12D	110.9
C5—C6—H6	120.1	C12^{ii}—C12'—H12D	91.2
C8—C7—C6	120.6 (3)	H12C—C12'—H12D	108.9
C8—C7—H7	119.7	C1—N1—C3	104.5 (3)
C6—C7—H7	119.7	C1—N1—Cu1	127.1 (2)
C7—C8—C9	120.0 (3)	C3—N1—Cu1	127.8 (2)
C7—C8—H8	120.0	C1—N2—C2	107.0 (3)
C9—C8—H8	120.0	C1—N2—C11	133.1 (4)
C8—C9—C10	119.8 (3)	C2—N2—C11	115.7 (4)
C8—C9—H9	120.1	C1—N2—C11'	121.5 (4)
C10—C9—H9	120.1	C2—N2—C11'	127.7 (4)
C5—C10—C9	120.7 (3)	C4—O2—Cu1	108.55 (18)
C5—C10—H10	119.7	C12^{ii}—O3—C12'	87.8 (7)
C9—C10—H10	119.7	C12'—O3—C12^{ii}	114.1 (8)
C12—C11—N2	101.3 (8)	C12^{ii}—O3—C12	114.1 (8)
C12—C11—H11A	111.5	C12^{ii}—O3—C12	148.0 (9)
N2—C11—H11A	111.5		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1A···O1^{iii}	0.85 (4)	2.08 (5)	2.862 (3)	153 (4)

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

Fig. 1

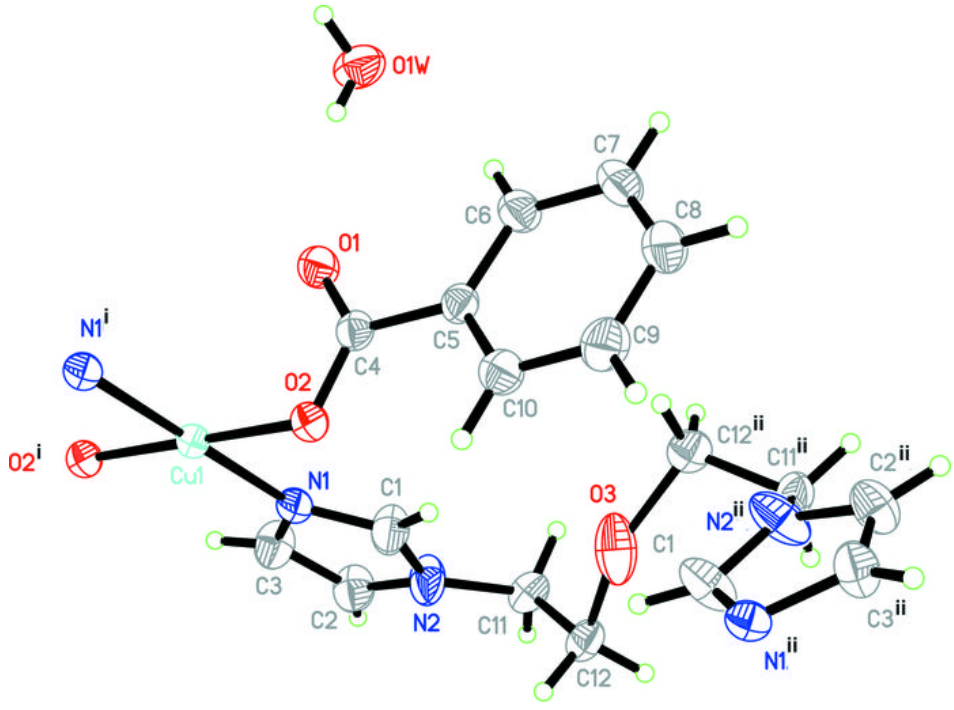
O1W
C7
C6
C8
O1
N1i
C5
C9
C4
O2
C10
C12ii
C11ii
C2ii
O2i
Cu1
N1
C1
O3
N2ii
C1
C3
C2
N2
C11
C3ii
N1ii
C12

Fig. 2

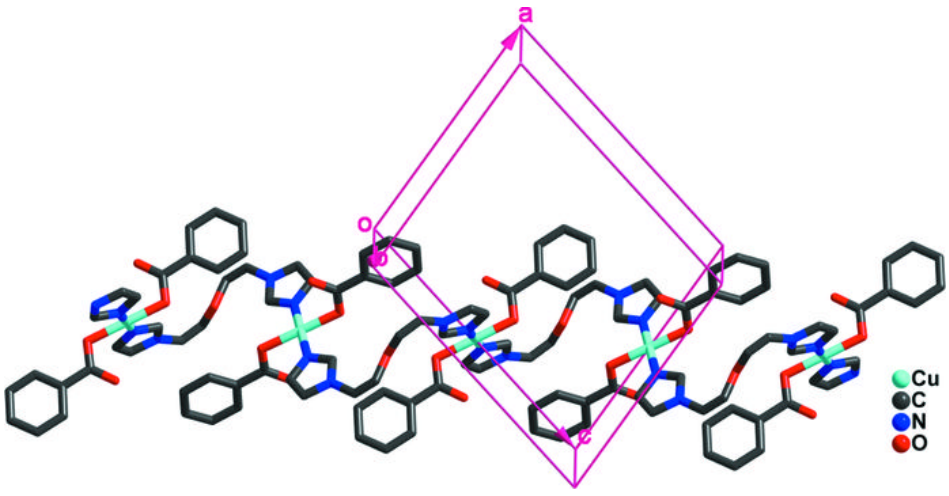

Fig. 3