

# catena-Poly[[[(4,7-dimethyl-1,10-phenanthroline- $\kappa^2N,N'$ )(formato- $\kappa O$ )-copper(II)]- $\mu$ -formato- $\kappa^2 O:O'$ ] mono-hydrate]

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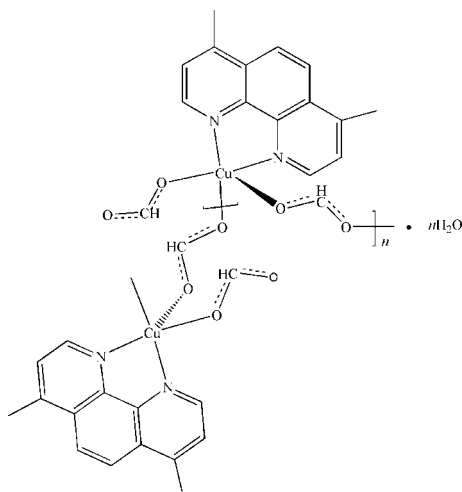
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Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(C-C) = 0.005$  Å;  $R$  factor = 0.042;  $wR$  factor = 0.104; data-to-parameter ratio = 16.4.

The title compound,  $[Cu(CHO_2)_2(C_{14}H_{12}N_2)] \cdot H_2O$ , consists of solvent water molecules and one-dimensional  $[Cu(dmph)(HCOO)(\mu-HCOO)_{2/2}]_n$  polymeric chains ( $dmph = 4,7$ -dimethyl-1,10-phenanthroline). The polymeric chains are generated from the  $[Cu(dmph)(HCOO)]^+$  units bridged by formate anions. The Cu atom is coordinated in a square-pyramidal environment. Interdigitation of the polymeric chains results in two-dimensional layers, which are stabilized by interchain  $\pi$ - $\pi$  stacking interactions (mean 3.53 Å). The supramolecular assembly of the resulting layers is accomplished by interlayer C-H...O hydrogen-bonding interactions.

## Related literature

For related literature, see: Chen & Suslick (1993); Hoskins & Robson (1990); Kondo *et al.* (1997); Maruoka *et al.* (1993); Sheldrick (1990).



## Experimental

### Crystal data

$[Cu(CHO_2)_2(C_{14}H_{12}N_2)] \cdot H_2O$   
 $M_r = 379.85$   
Monoclinic,  $C2/c$   
 $a = 21.260$  (4) Å  
 $b = 7.5010$  (15) Å  
 $c = 20.819$  (4) Å  
 $\beta = 109.17$  (3)°  
 $V = 3135.9$  (11) Å<sup>3</sup>  
 $Z = 8$   
Mo  $K\alpha$  radiation  
 $\mu = 1.42$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
 $0.49 \times 0.42 \times 0.20$  mm

### Data collection

Bruker P4 diffractometer  
Absorption correction: multi-scan (*XSCANS*; Siemens, 1996)  
 $T_{min} = 0.514$ ,  $T_{max} = 0.758$   
4506 measured reflections  
3610 independent reflections  
2545 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.026$   
3 standard reflections every 97 reflections  
intensity decay: none

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.104$   
 $S = 1.01$   
3610 reflections  
220 parameters  
 $\Delta\rho_{max} = 0.29$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.37$  e Å<sup>-3</sup>  
H atoms treated by a mixture of independent and constrained refinement

Table 1

Selected geometric parameters (Å, °).

Cu—O1	1.925 (2)	Cu—N1	2.010 (2)
Cu—O3 <sup>i</sup>	1.959 (2)	Cu—O4	2.236 (2)
Cu—N2	2.002 (2)		
O1—Cu—O3 <sup>i</sup>	94.67 (10)	N2—Cu—N1	81.30 (10)
O1—Cu—N2	91.45 (10)	O1—Cu—O4	98.72 (10)
O3 <sup>i</sup> —Cu—N2	163.53 (10)	O3 <sup>i</sup> —Cu—O4	93.07 (9)
O1—Cu—N1	165.67 (10)	N2—Cu—O4	101.11 (9)
O3 <sup>i</sup> —Cu—N1	89.27 (10)	N1—Cu—O4	94.82 (9)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O5—H5A...O2	0.841	2.070	2.872 (5)	158
O5—H5B...O4 <sup>ii</sup>	0.817	2.090	2.899 (6)	172
C1—H1...O3 <sup>iii</sup>	0.93	2.52	2.986 (2)	111
C2—H2...O2 <sup>iv</sup>	0.93	2.52	3.422 (4)	162
C9—H9...O5 <sup>v</sup>	0.93	2.34	3.220 (5)	157
C10—H10...O1	0.93	2.56	3.026 (3)	111
C15—H15...O1 <sup>vi</sup>	0.93	2.45	3.002 (3)	118
C15—H15...O3 <sup>iii</sup>	0.93	2.50	3.057 (5)	119

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

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: BQ2034).

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**supplementary materials**

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***catena-Poly[[[(4,7-dimethyl-1,10-phenanthroline- $\kappa^2N,N'$ )(formato- $\kappa O$ )copper(II)]- $\mu$ -formato- $\kappa^2O:O'$ ] monohydrate]***

**J.-L. Lin, X.-K. Qiu and Y.-Q. Zheng**

**Comment**

Metal–organic coordination complexes containing the aliphatic carboxylic acid ligand has been studied extensively due to their wide range of applications (Maruoka *et al.*, 1993; Chen & Suslick, 1993; Hoskins & Robson, 1990; Kondo *et al.*, 1997). Here, we report the crystal structure of one such complex, the title compound, (I).

The molecular structure of (I) is illustrated in Fig. 1. The asymmetric unit of (I) contains a  $\text{Cu}_{2+}$  ion, a 4,7-dimethyl-1,10-phenanthroline (dmph) molecule, two formate ions and a  $\text{H}_2\text{O}$  molecule. As depicted in Fig. 1, two crystallographically distinct formate ions are bonded to Cu atoms in different coordination modes, one being a monodentate ligand in an *syn* fashion and the other bidentate one bridging two Cu atoms in an anti-anti fashion with the one end axially bonded to one Cu atom and the other end equatorially approaching the other metal atom. The Cu atoms are coordinated by two N atoms of one dmph ligand and three O atoms of different formate anions to complete square pyramidal  $\text{CuN}_2\text{O}_3$  chromophore with one oxygen atom of one bidentate formate anion at the apex. The Cu atom is found to be displaced by 0.237 Å from the basal plane towards the apical O4 atom. Through the bidentate formate anions, the  $[\text{Cu}(\text{dmph})(\text{HCO}_2)]_n$  units are bridged to generate infinite chains formulated as  $[\text{Cu}(\text{dmph})(\text{HCO}_2)(\mu\text{-HCO}_2)_{2/2}]_n$ . The resulting chains extend along the crystallographic *b* axis with the dmph ligands pendent on both sides and the lattice water molecules are attached to the chains by forming hydrogen bonds to the uncoordinating formate oxygen atom as well as to the axially coordinated formate oxygen atom. The dmph ligands of one polymeric chain are each sandwiched by two aromatic neighbors of adjacent chains and such interdigitation of the chains give two-dimensional layers parallel to (100) as shown in Fig. 2. The mean interplanar distance between interdigitating dmph ligands is 3.53 Å, indicating the resulting two-dimensional layers are stabilized by the interchain  $\pi$ - $\pi$  stacking interactions. The layers are stacked along the [100] and between them are present weak C—H $\cdots$ O hydrogen bonds, which result from the —CH groups on the aromatic ring donating hydrogen atoms to the uncoordinating formate oxygen atoms as well as to the water oxygen atoms. According to the above description, the interlayer C—H $\cdots$ O hydrogen bonding interactions are responsible for supramolecular assembly of the two-dimensional layers.

**Experimental**

1.0 ml (1 M)  $\text{Na}_2\text{CO}_3$  was dropwise added to a stirring aqueous solution of 0.110 g (0.442 mmol)  $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$  in 5.0 ml  $\text{H}_2\text{O}$ , yielding pale blue precipitate, which was separated by centrifugalization and washed with de-ionized  $\text{H}_2\text{O}$  until no detectable  $\text{SO}_4^{2-}$  ions in supernatant. The fresh precipitate was then added to a stirred methanolic aqueous solution of 0.100 g (0.442 mmol) 4,7-dimethyl-1,10-phenanthroline (dmph) in 20 ml  $\text{CH}_3\text{OH}/\text{H}_2\text{O}$  (*v/v* = 1:1). Under continuous stirring, 1.0 ml formic acid was added and the dark green suspension was filtered off. Slow evaporation of the dark green filtrate (pH = 3.55) at room temperature afforded a small amount of dark green prismatic crystals.

## Refinement

The H5A and H5B atoms of the aqua molecules were located from difference Fourier synthesis, with O—H distances refined. Other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 and 0.96 Å.

## Figures

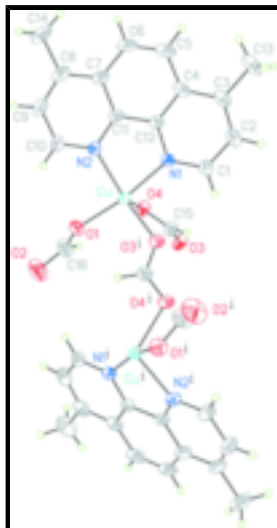


Fig. 1. The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. (I: 0.5-*X*, 0.5+*Y*, 0.5-*Z*)

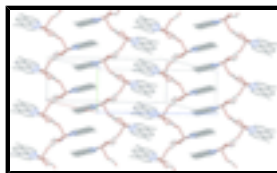


Fig. 2. A view of a single layer of (I). H atoms, solvent water molecules and hydrogen bonds have been omitted.

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### Crystal data

[Cu(CHO<sub>2</sub>)<sub>2</sub>(C<sub>14</sub>H<sub>12</sub>N<sub>2</sub>)]·H<sub>2</sub>O

*M<sub>r</sub>* = 379.85

Monoclinic, *C2/c*

Hall symbol: -*C* 2yc

*a* = 21.260 (4) Å

*b* = 7.5010 (15) Å

*c* = 20.819 (4) Å

$\beta$  = 109.17 (3)°

*V* = 3135.9 (11) Å<sup>3</sup>

*Z* = 8

*F*<sub>000</sub> = 1560

*D<sub>x</sub>* = 1.609 Mg m<sup>-3</sup>

Mo *K*α radiation

$\lambda$  = 0.71073 Å

Cell parameters from 25 reflections

$\theta$  = 5.0–12.5°

$\mu$  = 1.42 mm<sup>-1</sup>

*T* = 295 (2) K

Block, blue

0.49 × 0.42 × 0.20 mm

*Data collection*

Bruker P4 diffractometer	$R_{\text{int}} = 0.026$
Radiation source: fine-focus sealed tube	$\theta_{\text{max}} = 27.5^\circ$
Monochromator: graphite	$\theta_{\text{min}} = 2.0^\circ$
$T = 295(2)$ K	$h = -27 \rightarrow 1$
$\theta/2\theta$ scans	$k = -1 \rightarrow 9$
Absorption correction: empirical (using intensity measurements)	$l = -25 \rightarrow 27$
XSCANS (Siemens, 1996)	
$T_{\text{min}} = 0.514$ , $T_{\text{max}} = 0.758$	3 standard reflections
4506 measured reflections	every 97 reflections
3610 independent reflections	intensity decay: none
2545 reflections with $I > 2\sigma(I)$	

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.104$	$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 3.5441P]$
$S = 1.01$	where $P = (F_o^2 + 2F_c^2)/3$
3610 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
220 parameters	$\Delta\rho_{\text{max}} = 0.29 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.37 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

*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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu	0.210963 (17)	0.14358 (5)	0.138649 (17)	0.03511 (13)
N1	0.28595 (12)	0.0478 (3)	0.10998 (11)	0.0343 (5)

## supplementary materials

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N2	0.16109 (12)	0.1064 (3)	0.03976 (12)	0.0382 (6)
C1	0.34873 (15)	0.0172 (5)	0.14787 (16)	0.0430 (8)
H1	0.3616	0.0384	0.1944	0.066 (4)*
C2	0.39574 (17)	-0.0458 (5)	0.12009 (19)	0.0532 (9)
H2	0.4390	-0.0674	0.1485	0.066 (4)*
C3	0.37948 (18)	-0.0761 (5)	0.05218 (19)	0.0503 (9)
C4	0.31229 (17)	-0.0472 (4)	0.01027 (16)	0.0434 (8)
C5	0.2868 (2)	-0.0771 (5)	-0.06134 (18)	0.0563 (10)
H5	0.3152	-0.1194	-0.0837	0.066 (4)*
C6	0.2223 (2)	-0.0452 (5)	-0.09741 (16)	0.0556 (10)
H6	0.2076	-0.0655	-0.1441	0.066 (4)*
C7	0.17582 (18)	0.0183 (4)	-0.06652 (15)	0.0447 (8)
C8	0.10791 (19)	0.0569 (5)	-0.10138 (16)	0.0541 (9)
C9	0.07013 (19)	0.1179 (5)	-0.06408 (17)	0.0596 (10)
H9	0.0254	0.1439	-0.0858	0.066 (4)*
C10	0.09741 (17)	0.1416 (5)	0.00558 (16)	0.0496 (8)
H10	0.0703	0.1837	0.0294	0.066 (4)*
C11	0.19947 (15)	0.0465 (4)	0.00405 (14)	0.0359 (7)
C12	0.26794 (15)	0.0136 (4)	0.04252 (14)	0.0352 (7)
C13	0.4312 (2)	-0.1361 (6)	0.0215 (2)	0.0773 (13)
H13A	0.4743	-0.1361	0.0559	0.116*
H13B	0.4314	-0.0561	-0.0144	0.116*
H13C	0.4207	-0.2543	0.0035	0.116*
C14	0.0778 (2)	0.0341 (7)	-0.17721 (17)	0.0812 (14)
H14A	0.0340	0.0855	-0.1925	0.122*
H14B	0.0749	-0.0906	-0.1882	0.122*
H14C	0.1053	0.0927	-0.1993	0.122*
O1	0.13880 (11)	0.2811 (3)	0.14987 (11)	0.0510 (6)
O2	0.05869 (16)	0.3299 (5)	0.19201 (18)	0.0922 (11)
C15	0.23199 (16)	-0.1615 (5)	0.23724 (16)	0.0450 (8)
H15	0.2727	-0.1026	0.2512	0.066 (4)*
O3	0.22397 (11)	-0.2789 (3)	0.27525 (11)	0.0495 (6)
O4	0.19140 (11)	-0.1144 (3)	0.18250 (10)	0.0484 (6)
C16	0.09874 (19)	0.2349 (6)	0.1778 (2)	0.0637 (11)
H16	0.0990	0.1150	0.1893	0.066 (4)*
O5	0.06640 (15)	0.6969 (5)	0.1560 (2)	0.1152 (14)
H5A	0.0635	0.5850	0.1555	0.120*
H5B	0.1033	0.7409	0.1635	0.120*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu	0.0352 (2)	0.0401 (2)	0.02959 (18)	0.00407 (18)	0.01001 (14)	-0.00091 (17)
N1	0.0356 (13)	0.0347 (14)	0.0332 (12)	0.0012 (12)	0.0119 (10)	0.0004 (11)
N2	0.0397 (14)	0.0402 (15)	0.0320 (12)	0.0043 (12)	0.0081 (11)	0.0027 (11)
C1	0.0354 (17)	0.0459 (19)	0.0461 (17)	0.0012 (15)	0.0114 (14)	0.0007 (15)
C2	0.0358 (18)	0.053 (2)	0.072 (2)	0.0016 (17)	0.0201 (17)	0.000 (2)
C3	0.053 (2)	0.0385 (18)	0.073 (2)	0.0006 (16)	0.0396 (19)	-0.0017 (18)

C4	0.057 (2)	0.0319 (18)	0.0519 (18)	-0.0009 (16)	0.0329 (16)	-0.0004 (15)
C5	0.084 (3)	0.047 (2)	0.053 (2)	-0.006 (2)	0.044 (2)	-0.0059 (18)
C6	0.092 (3)	0.048 (2)	0.0343 (16)	-0.006 (2)	0.0303 (19)	-0.0022 (16)
C7	0.064 (2)	0.0357 (17)	0.0315 (14)	-0.0048 (16)	0.0117 (15)	0.0005 (14)
C8	0.071 (2)	0.046 (2)	0.0334 (16)	-0.0072 (19)	0.0008 (16)	0.0048 (16)
C9	0.052 (2)	0.061 (3)	0.0476 (19)	0.0043 (19)	-0.0076 (17)	0.0050 (18)
C10	0.0460 (18)	0.051 (2)	0.0441 (17)	0.0126 (17)	0.0046 (14)	0.0039 (17)
C11	0.0476 (17)	0.0303 (16)	0.0294 (13)	-0.0031 (14)	0.0122 (13)	0.0018 (13)
C12	0.0420 (17)	0.0322 (16)	0.0327 (14)	-0.0027 (14)	0.0142 (13)	0.0023 (13)
C13	0.072 (3)	0.075 (3)	0.110 (3)	0.007 (2)	0.063 (3)	-0.001 (3)
C14	0.102 (3)	0.087 (3)	0.0343 (17)	-0.004 (3)	-0.006 (2)	-0.002 (2)
O1	0.0474 (13)	0.0567 (15)	0.0531 (13)	0.0103 (12)	0.0222 (11)	0.0009 (12)
O2	0.071 (2)	0.110 (3)	0.114 (3)	0.0250 (19)	0.057 (2)	0.007 (2)
C15	0.0428 (18)	0.0456 (19)	0.0448 (17)	0.0007 (15)	0.0119 (15)	0.0096 (16)
O3	0.0497 (13)	0.0542 (14)	0.0396 (11)	-0.0064 (12)	0.0077 (10)	0.0149 (11)
O4	0.0510 (13)	0.0515 (15)	0.0383 (11)	-0.0002 (11)	0.0088 (10)	0.0147 (10)
C16	0.052 (2)	0.073 (3)	0.074 (3)	0.012 (2)	0.032 (2)	0.009 (2)
O5	0.0537 (19)	0.093 (3)	0.167 (4)	0.0016 (19)	-0.006 (2)	0.014 (3)

*Geometric parameters (Å, °)*

Cu—O1	1.925 (2)	C7—C8	1.417 (5)
Cu—O3 <sup>i</sup>	1.959 (2)	C8—C9	1.367 (5)
Cu—N2	2.002 (2)	C8—C14	1.506 (4)
Cu—N1	2.010 (2)	C9—C10	1.385 (5)
Cu—O4	2.236 (2)	C9—H9	0.9300
N1—C1	1.329 (4)	C10—H10	0.9300
N1—C12	1.353 (3)	C11—C12	1.434 (4)
N2—C10	1.333 (4)	C13—H13A	0.9600
N2—C11	1.349 (4)	C13—H13B	0.9600
C1—C2	1.391 (4)	C13—H13C	0.9600
C1—H1	0.9300	C14—H14A	0.9600
C2—C3	1.360 (5)	C14—H14B	0.9600
C2—H2	0.9300	C14—H14C	0.9600
C3—C4	1.425 (5)	O1—C16	1.228 (4)
C3—C13	1.510 (5)	O2—C16	1.219 (5)
C4—C12	1.401 (4)	C15—O3	1.232 (4)
C4—C5	1.427 (5)	C15—O4	1.234 (4)
C5—C6	1.351 (5)	C15—H15	0.9300
C5—H5	0.9300	O3—Cu <sup>ii</sup>	1.959 (2)
C6—C7	1.426 (5)	C16—H16	0.9300
C6—H6	0.9300	O5—H5A	0.8414
C7—C11	1.404 (4)	O5—H5B	0.8169
O1—Cu—O3 <sup>i</sup>	94.67 (10)	C9—C8—C7	117.9 (3)
O1—Cu—N2	91.45 (10)	C9—C8—C14	120.5 (4)
O3 <sup>i</sup> —Cu—N2	163.53 (10)	C7—C8—C14	121.6 (4)
O1—Cu—N1	165.67 (10)	C8—C9—C10	121.1 (3)
O3 <sup>i</sup> —Cu—N1	89.27 (10)	C8—C9—H9	119.5



## supplementary materials

N2—Cu—N1	81.30 (10)	C10—C9—H9	119.5
O1—Cu—O4	98.72 (10)	N2—C10—C9	122.4 (3)
O3 <sup>i</sup> —Cu—O4	93.07 (9)	N2—C10—H10	118.8
N2—Cu—O4	101.11 (9)	C9—C10—H10	118.8
N1—Cu—O4	94.82 (9)	N2—C11—C7	123.6 (3)
C1—N1—C12	118.0 (3)	N2—C11—C12	115.9 (2)
C1—N1—Cu	128.7 (2)	C7—C11—C12	120.5 (3)
C12—N1—Cu	113.22 (19)	N1—C12—C4	123.6 (3)
C10—N2—C11	117.6 (3)	N1—C12—C11	115.9 (2)
C10—N2—Cu	128.6 (2)	C4—C12—C11	120.5 (3)
C11—N2—Cu	113.7 (2)	C3—C13—H13A	109.5
N1—C1—C2	122.1 (3)	C3—C13—H13B	109.5
N1—C1—H1	119.0	H13A—C13—H13B	109.5
C2—C1—H1	119.0	C3—C13—H13C	109.5
C3—C2—C1	121.1 (3)	H13A—C13—H13C	109.5
C3—C2—H2	119.4	H13B—C13—H13C	109.5
C1—C2—H2	119.4	C8—C14—H14A	109.5
C2—C3—C4	118.2 (3)	C8—C14—H14B	109.5
C2—C3—C13	121.2 (4)	H14A—C14—H14B	109.5
C4—C3—C13	120.6 (3)	C8—C14—H14C	109.5
C12—C4—C3	117.0 (3)	H14A—C14—H14C	109.5
C12—C4—C5	117.9 (3)	H14B—C14—H14C	109.5
C3—C4—C5	125.2 (3)	C16—O1—Cu	127.6 (3)
C6—C5—C4	121.4 (3)	O3—C15—O4	126.5 (3)
C6—C5—H5	119.3	O3—C15—H15	116.7
C4—C5—H5	119.3	O4—C15—H15	116.7
C5—C6—C7	122.4 (3)	C15—O3—Cu <sup>ii</sup>	126.5 (2)
C5—C6—H6	118.8	C15—O4—Cu	117.2 (2)
C7—C6—H6	118.8	O2—C16—O1	126.8 (4)
C11—C7—C8	117.4 (3)	O2—C16—H16	116.6
C11—C7—C6	117.3 (3)	O1—C16—H16	116.6
C8—C7—C6	125.3 (3)	H5A—O5—H5B	117.9

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

### Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O5—H5A $\cdots$ O2	0.841	2.070	2.872 (5)	158
O5—H5B $\cdots$ O4 <sup>iii</sup>	0.817	2.090	2.899 (6)	172
C1—H1 $\cdots$ O3 <sup>iv</sup>	0.93	2.52	2.986 (2)	111
C2—H2 $\cdots$ O2 <sup>v</sup>	0.93	2.52	3.422 (4)	162
C9—H9 $\cdots$ O5 <sup>vi</sup>	0.93	2.34	3.220 (5)	157
C10—H10 $\cdots$ O1	0.93	2.56	3.026 (3)	111
C15—H15 $\cdots$ O1 <sup>ii</sup>	0.93	2.45	3.002 (3)	118
C15—H15 $\cdots$ O3 <sup>iv</sup>	0.93	2.50	3.057 (5)	119

Symmetry codes: (iii)  $x, y+1, z$ ; (iv)  $-x+1/2, y+1/2, -z+1/2$ ; (v)  $x+1/2, y-1/2, z$ ; (vi)  $-x, -y+1, -z$ ; (ii)  $-x+1/2, y-1/2, -z+1/2$ .

Fig. 1

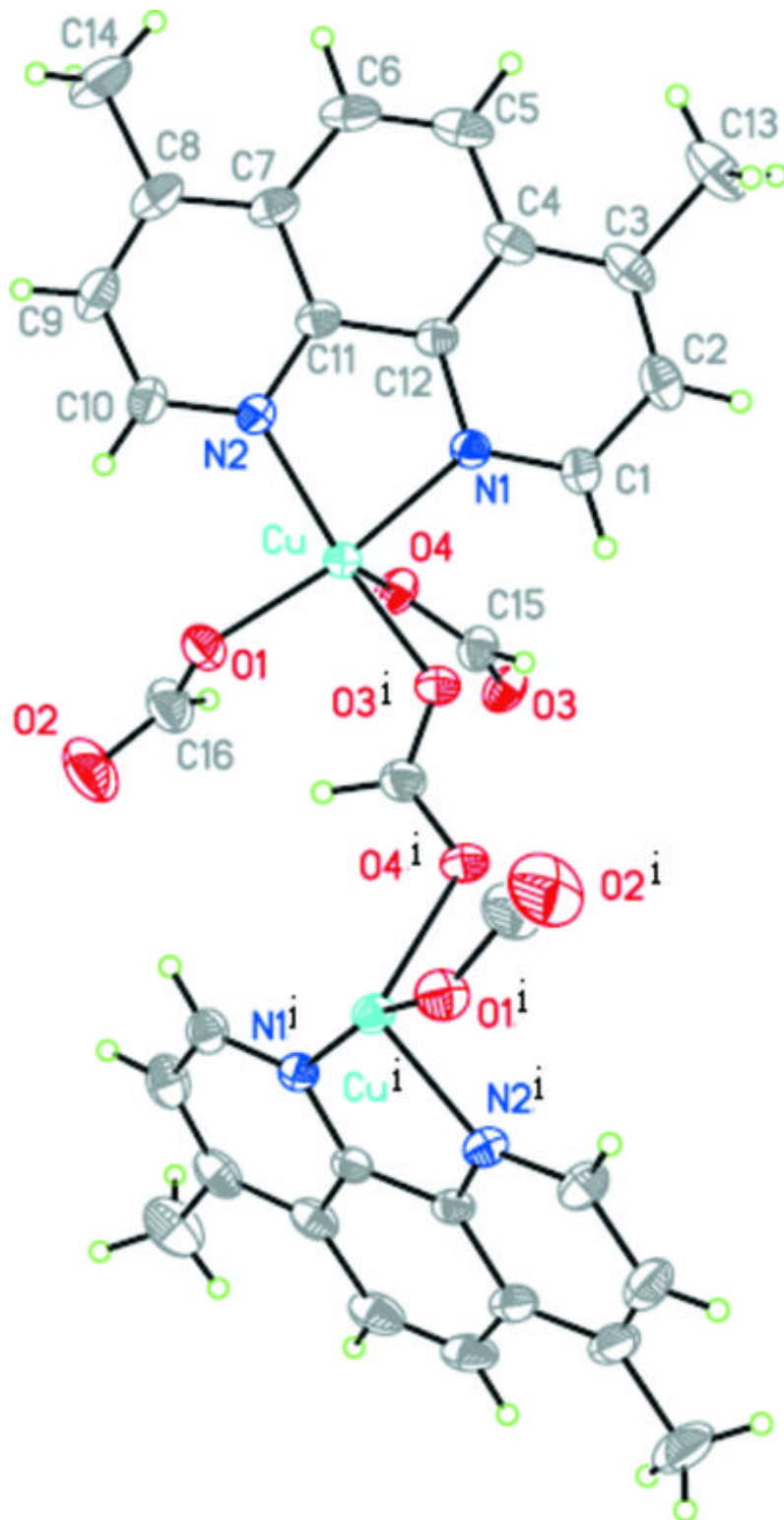


Fig. 2

