

Poly[[*(N,N*-dimethylformamide- κ O)(μ_3 -pyrazine-2,3-dicarboxylato- $\kappa^4N^1,O^2:O^3:O^3$)copper(II)] monohydrate]

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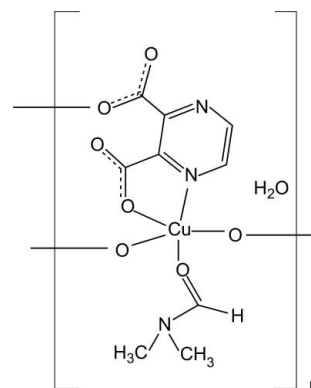
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.051; wR factor = 0.115; data-to-parameter ratio = 12.7.

In the title compound, $\{[\text{Cu}(\text{C}_6\text{H}_2\text{N}_2\text{O}_4)(\text{C}_3\text{H}_7\text{NO})]\cdot\text{H}_2\text{O}\}_n$, the Cu(II) atom is coordinated by an *N,O*-bidentate pyrazine-2,3-dicarboxylate (pzdc) dianion, two O atoms from two other pzdc anions and one O atom from the dimethylformamide ligand, forming a distorted square-pyramidal CuNO_4 geometry. The polymeric character of the structure is established by the formation of layers parallel to (100) via bridging pzdc ligands. O—H...O hydrogen bonding between water molecules and uncoordinated carboxylate O atoms leads to additional stabilization of the structure.

Related literature

For related structures with the pyrazine-2,3-dicarboxylate (pzdc) dianion, see: Hua & Liu (2009); Konar *et al.* (2004); Li *et al.* (2004); Lin *et al.* (2009); Tombul & Guven (2009); Wang *et al.* (2008); Xiang *et al.* (2004); Xu *et al.* (2008).



Experimental

Crystal data

$[\text{Cu}(\text{C}_6\text{H}_2\text{N}_2\text{O}_4)(\text{C}_3\text{H}_7\text{NO})]\cdot\text{H}_2\text{O}$
 $M_r = 320.75$
Monoclinic, $P2_1/c$
 $a = 10.1656$ (5) Å
 $b = 13.6310$ (8) Å
 $c = 9.1461$ (2) Å
 $\beta = 91.430$ (2)°

$V = 1266.96$ (10) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 1.75$ mm⁻¹
 $T = 298$ K
 $0.39 \times 0.10 \times 0.06$ mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: integration (*SADABS*; Bruker, 2002)
 $T_{\min} = 0.549$, $T_{\max} = 0.902$

6222 measured reflections
2283 independent reflections
1600 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.058$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.115$
 $S = 0.98$
2283 reflections
180 parameters
3 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.48$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.34$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O6}-\text{H6B}\cdots\text{O4}^{\text{i}}$	0.82 (5)	2.00 (3)	2.771 (5)	156 (7)
$\text{O6}-\text{H6A}\cdots\text{O1}^{\text{ii}}$	0.82 (5)	2.38 (3)	3.138 (6)	153 (5)
$\text{O6}-\text{H6A}\cdots\text{O2}^{\text{ii}}$	0.82 (5)	2.30 (3)	3.037 (5)	149 (5)

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: WM2283).

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supplementary materials

Acta Cryst. (2010). E66, m10-m11 [doi:10.1107/S1600536809051332]

Poly[[*N,N*-dimethylformamide- κ O](μ_3 -pyrazine-2,3-dicarboxylato- κ^4 N¹,O²:O³:O³)copper(II)] monohydrate]

Z.-Z. Fan, G.-P. Wang and Y.-S. Li

Comment

Polymeric compounds play an important role in the field of molecular magnetism. Di- and polycarboxylates are capable of bridging and providing effective magnetic exchange pathways. Pyrazine-2,3-dicarboxylic acid (H₂pzdc) has been widely applied to construct polymeric coordination compounds; their structures and magnetic properties were investigated (Li *et al.*, 2004; Xiang *et al.*, 2004; Hua & Liu, 2009; Lin *et al.*, 2009; Tombul & Guven, 2009). We present here the structure of the title compound, {[Cu(pzdc)(DMF)]H₂O}_n, (I).

In the structure of compound (I), each Cu(II) atom is coordinated by an N atom of the pyrazine ring and a carboxylic O atom from one pzdc²⁻ anion, two O atoms from two other pzdc²⁻ anions, and O atom from DMF, forming a distorted square-pyramidal environment, as depicted in Fig. 1. The four atoms N1, O2, O5 and O3ⁱ form the basal plane, whereas the O3ⁱⁱ atom [symmetry code: (i) $-x+1, y-1/2, -z+1$; (ii) $x, -y+3/2, z-1/2$] occupies the apical site with a longer Cu1—O3ⁱⁱ bond length of 2.378 (3) Å. In the basal plane, the bond distances of Cu1—N1 and Cu1—O3ⁱ are 2.002 (3) and 1.958 (3) Å, which are shorter than those observed for the distorted square-pyramidal CuN₂O₃ coordination in a related structure of a Cu(II)pzdc derivative (Hua & Liu, 2009). The plane defined by carboxylic group O1—C1—C2—C3 is nearly coplanar to the pyrazine ring with the dihedral angle of 3.7 (7)°, while another carboxylate plane defined by the C2—C3—C6—O4 is approximately perpendicular to the pyrazine ring [dihedral angle of 92.9 (5)°]. This conformation was also observed in a series of other transition metal complexes formed with H₂pzdc (Li *et al.*, 2004; Xiang *et al.*, 2004; Konar *et al.*, 2004; Hua *et al.*, 2009). Extensive hydrogen bonding interactions help to stabilize the structure. The carboxylate O atoms take part in a O—H...O hydrogen bonding and are acceptor atoms with O atoms of water molecules as donor atoms (Table 1).

Experimental

Mixed DMF and aqueous solution (15 ml) of CuCl₂·2H₂O (0.5 mmol) and 2,3-pyrazinedicarboxylic acid (H₂pzdc, 0.25 mmol) were slowly added into a methanolic (5 ml) solution of triethylene diamine (TED, 0.5 mmol); the resulting mixture was stirred for 5 minutes and allowed to stand at room temperature for about four days until blue single crystals were obtained.

Refinement

H atoms of the water molecules were located in a difference Fourier map and were refined isotropically, with O—H and H—H distance restraints of 0.84 (1) Å and 1.37 (2) Å, respectively. The remaining H atoms were positioned geometrically (C—H = 0.93 Å) and allowed to ride on their parent atoms. The $U_{\text{iso}}(\text{H})$ values were set at $1.2U_{\text{eq}}(\text{C})$ and $1.5U_{\text{eq}}(\text{O})$.

Figures

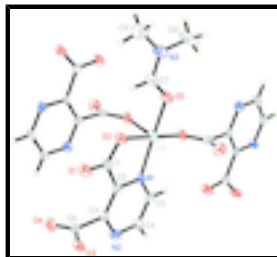


Fig. 1. The coordination of the Cu(II) atom in the structure of compound (I), showing atom labels and 50% probability displacement ellipsoids for the non-H atoms.

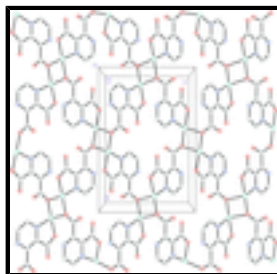


Fig. 2. The polymeric structure of compound (I); water molecules and DMF have been omitted for clarity.

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Crystal data

[Cu(C₆H₂N₂O₄)(C₃H₇NO)]·H₂O

$M_r = 320.75$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.1656$ (5) Å

$b = 13.6310$ (8) Å

$c = 9.1461$ (2) Å

$\beta = 91.430$ (2)°

$V = 1266.96$ (10) Å³

$Z = 4$

$F(000) = 652$

$D_x = 1.682$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1111 reflections

$\theta = 2.5$ – 22.4 °

$\mu = 1.75$ mm⁻¹

$T = 298$ K

Prism, blue

$0.39 \times 0.10 \times 0.06$ mm

Data collection

Bruker APEX area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

phi and ω scans

Absorption correction: integration (*SADABS*; Bruker, 2002)

$T_{\min} = 0.549$, $T_{\max} = 0.902$

6222 measured reflections

2283 independent reflections

1600 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.058$

$\theta_{\text{max}} = 25.3$ °, $\theta_{\text{min}} = 2.0$ °

$h = -8 \rightarrow 12$

$k = -16 \rightarrow 16$

$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.051$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.115$	H atoms treated by a mixture of independent and constrained refinement
$S = 0.98$	$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2]$
2283 reflections	where $P = (F_o^2 + 2F_c^2)/3$
180 parameters	$(\Delta/\sigma)_{\max} < 0.001$
3 restraints	$\Delta\rho_{\max} = 0.48 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.34 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.59999 (5)	0.58784 (3)	0.07521 (6)	0.0402 (2)
O1	0.5775 (3)	0.8747 (2)	0.1085 (4)	0.0526 (10)
O2	0.6295 (3)	0.7254 (2)	0.0382 (4)	0.0463 (9)
O3	0.4380 (3)	0.9489 (2)	0.3914 (3)	0.0386 (8)
O4	0.2821 (3)	0.9362 (2)	0.2189 (4)	0.0511 (9)
O5	0.7494 (3)	0.5510 (2)	-0.0435 (4)	0.0503 (9)
O6	0.2218 (5)	0.1287 (3)	0.1467 (7)	0.121 (2)
N1	0.4710 (3)	0.6417 (2)	0.2162 (4)	0.0298 (8)
N2	0.3001 (3)	0.7442 (2)	0.3914 (4)	0.0402 (9)
N3	0.9066 (4)	0.5894 (4)	-0.2048 (5)	0.0655 (13)
C1	0.5654 (4)	0.7859 (3)	0.1145 (5)	0.0331 (10)
C2	0.4684 (4)	0.7404 (3)	0.2158 (4)	0.0279 (9)
C3	0.3821 (4)	0.7913 (3)	0.3018 (5)	0.0316 (10)
C4	0.3064 (4)	0.6467 (3)	0.3912 (5)	0.0420 (12)
H4	0.2516	0.6118	0.4523	0.050*
C5	0.3912 (4)	0.5951 (3)	0.3039 (5)	0.0381 (11)
H5	0.3920	0.5269	0.3071	0.046*

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C6	0.3670 (4)	0.9018 (3)	0.3005 (5)	0.0352 (10)
C7	0.8054 (5)	0.6097 (4)	-0.1238 (6)	0.0554 (14)
H7	0.7732	0.6735	-0.1271	0.066*
C8	0.9664 (6)	0.6630 (5)	-0.2983 (8)	0.112 (3)
H8A	0.9216	0.7244	-0.2874	0.168*
H8B	0.9593	0.6421	-0.3985	0.168*
H8C	1.0575	0.6707	-0.2706	0.168*
C9	0.9607 (6)	0.4924 (5)	-0.2062 (7)	0.092 (2)
H9A	1.0486	0.4937	-0.1655	0.137*
H9B	0.9624	0.4688	-0.3051	0.137*
H9C	0.9073	0.4496	-0.1491	0.137*
H6A	0.277 (5)	0.148 (4)	0.089 (6)	0.110*
H6B	0.219 (6)	0.0685 (9)	0.155 (7)	0.110*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0472 (4)	0.0182 (3)	0.0560 (4)	0.0032 (2)	0.0188 (3)	0.0026 (3)
O1	0.075 (2)	0.0191 (15)	0.065 (3)	-0.0083 (15)	0.029 (2)	-0.0011 (16)
O2	0.0559 (19)	0.0221 (15)	0.062 (2)	-0.0013 (14)	0.0282 (17)	0.0013 (16)
O3	0.0467 (17)	0.0189 (14)	0.050 (2)	-0.0034 (13)	0.0072 (16)	-0.0062 (15)
O4	0.060 (2)	0.0361 (18)	0.057 (2)	0.0112 (16)	-0.0027 (19)	-0.0003 (17)
O5	0.047 (2)	0.0345 (17)	0.070 (3)	0.0050 (15)	0.0268 (18)	0.0034 (17)
O6	0.102 (4)	0.071 (3)	0.192 (6)	0.010 (3)	0.078 (4)	0.054 (4)
N1	0.0353 (19)	0.0157 (17)	0.039 (2)	-0.0021 (14)	0.0026 (17)	0.0003 (16)
N2	0.049 (2)	0.029 (2)	0.043 (2)	-0.0043 (17)	0.0103 (19)	-0.0032 (18)
N3	0.041 (2)	0.083 (3)	0.074 (4)	0.010 (2)	0.021 (2)	0.004 (3)
C1	0.040 (2)	0.025 (2)	0.034 (3)	-0.0004 (19)	0.008 (2)	-0.002 (2)
C2	0.036 (2)	0.019 (2)	0.029 (3)	-0.0042 (17)	-0.0021 (19)	-0.0008 (18)
C3	0.038 (2)	0.025 (2)	0.032 (3)	-0.0013 (18)	-0.001 (2)	-0.0019 (19)
C4	0.052 (3)	0.030 (2)	0.045 (3)	-0.010 (2)	0.011 (2)	0.002 (2)
C5	0.050 (3)	0.021 (2)	0.044 (3)	-0.004 (2)	0.007 (2)	0.000 (2)
C6	0.039 (2)	0.026 (2)	0.041 (3)	0.004 (2)	0.014 (2)	0.004 (2)
C7	0.043 (3)	0.053 (3)	0.070 (4)	0.009 (2)	0.005 (3)	-0.007 (3)
C8	0.072 (4)	0.144 (7)	0.121 (7)	0.014 (4)	0.049 (4)	0.053 (5)
C9	0.062 (4)	0.098 (5)	0.116 (6)	0.011 (4)	0.030 (4)	-0.050 (4)

Geometric parameters (\AA , $^\circ$)

Cu1—O2	1.930 (3)	N2—C3	1.346 (5)
Cu1—O5	1.954 (3)	N3—C7	1.313 (6)
Cu1—O3 ⁱ	1.958 (3)	N3—C9	1.432 (6)
Cu1—N1	2.002 (3)	N3—C8	1.460 (7)
Cu1—O3 ⁱⁱ	2.378 (3)	C1—C2	1.504 (5)
O1—C1	1.218 (5)	C2—C3	1.380 (5)
O2—C1	1.271 (5)	C3—C6	1.515 (5)
O3—C6	1.263 (5)	C4—C5	1.381 (6)
O3—Cu1 ⁱⁱⁱ	1.958 (3)	C4—H4	0.9300

O3—Cu1 ^{iv}	2.378 (3)	C5—H5	0.9300
O4—C6	1.220 (5)	C7—H7	0.9300
O5—C7	1.235 (6)	C8—H8A	0.9600
O6—H6A	0.82 (5)	C8—H8B	0.9600
O6—H6B	0.82 (5)	C8—H8C	0.9600
N1—C5	1.318 (5)	C9—H9A	0.9600
N1—C2	1.344 (4)	C9—H9B	0.9600
N2—C4	1.331 (5)	C9—H9C	0.9600
O2—Cu1—O5	91.48 (13)	C3—C2—C1	125.4 (4)
O2—Cu1—O3 ⁱ	177.39 (13)	N2—C3—C2	121.3 (4)
O5—Cu1—O3 ⁱ	89.82 (13)	N2—C3—C6	114.5 (4)
O2—Cu1—N1	82.17 (12)	C2—C3—C6	124.2 (4)
O5—Cu1—N1	169.37 (13)	N2—C4—C5	122.6 (4)
O3 ⁱ —Cu1—N1	96.87 (12)	N2—C4—H4	118.7
O2—Cu1—O3 ⁱⁱ	100.87 (12)	C5—C4—H4	118.7
O5—Cu1—O3 ⁱⁱ	94.99 (12)	N1—C5—C4	120.6 (4)
O3 ⁱ —Cu1—O3 ⁱⁱ	76.75 (12)	N1—C5—H5	119.7
N1—Cu1—O3 ⁱⁱ	94.57 (12)	C4—C5—H5	119.7
C1—O2—Cu1	116.7 (3)	O4—C6—O3	126.2 (4)
C6—O3—Cu1 ⁱⁱⁱ	118.9 (3)	O4—C6—C3	117.2 (4)
C6—O3—Cu1 ^{iv}	137.1 (3)	O3—C6—C3	116.4 (4)
Cu1 ⁱⁱⁱ —O3—Cu1 ^{iv}	103.25 (12)	O5—C7—N3	125.4 (5)
C7—O5—Cu1	122.7 (3)	O5—C7—H7	117.3
H6A—O6—H6B	113.5 (19)	N3—C7—H7	117.3
C5—N1—C2	118.1 (4)	N3—C8—H8A	109.5
C5—N1—Cu1	129.7 (3)	N3—C8—H8B	109.5
C2—N1—Cu1	112.2 (3)	H8A—C8—H8B	109.5
C4—N2—C3	116.4 (4)	N3—C8—H8C	109.5
C7—N3—C9	120.4 (5)	H8A—C8—H8C	109.5
C7—N3—C8	121.9 (5)	H8B—C8—H8C	109.5
C9—N3—C8	117.6 (5)	N3—C9—H9A	109.5
O1—C1—O2	124.5 (4)	N3—C9—H9B	109.5
O1—C1—C2	120.4 (4)	H9A—C9—H9B	109.5
O2—C1—C2	115.1 (3)	N3—C9—H9C	109.5
N1—C2—C3	121.0 (4)	H9A—C9—H9C	109.5
N1—C2—C1	113.7 (3)	H9B—C9—H9C	109.5
O5—Cu1—O2—C1	-169.1 (3)	O1—C1—C2—C3	3.7 (7)
O3 ⁱ —Cu1—O2—C1	71 (3)	O2—C1—C2—C3	-175.6 (4)
N1—Cu1—O2—C1	2.3 (3)	C4—N2—C3—C2	-0.4 (6)
O3 ⁱⁱ —Cu1—O2—C1	95.5 (3)	C4—N2—C3—C6	177.3 (4)
O2—Cu1—O5—C7	-11.7 (4)	N1—C2—C3—N2	1.5 (6)
O3 ⁱ —Cu1—O5—C7	166.0 (4)	C1—C2—C3—N2	-178.8 (4)
N1—Cu1—O5—C7	-64.7 (9)	N1—C2—C3—C6	-176.0 (4)
O3 ⁱⁱ —Cu1—O5—C7	89.4 (4)	C1—C2—C3—C6	3.7 (7)
O2—Cu1—N1—C5	179.2 (4)	C3—N2—C4—C5	-0.5 (6)

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O5—Cu1—N1—C5	-127.0 (7)	C2—N1—C5—C4	0.8 (6)
O3 ⁱ —Cu1—N1—C5	1.7 (4)	Cu1—N1—C5—C4	-178.4 (3)
O3 ⁱⁱ —Cu1—N1—C5	78.9 (4)	N2—C4—C5—N1	0.3 (7)
O2—Cu1—N1—C2	0.1 (3)	Cu1 ⁱⁱⁱ —O3—C6—O4	7.2 (6)
O5—Cu1—N1—C2	53.8 (8)	Cu1 ^{iv} —O3—C6—O4	175.4 (3)
O3 ⁱ —Cu1—N1—C2	-177.5 (3)	Cu1 ⁱⁱⁱ —O3—C6—C3	-167.7 (3)
O3 ⁱⁱ —Cu1—N1—C2	-100.3 (3)	Cu1 ^{iv} —O3—C6—C3	0.5 (6)
Cu1—O2—C1—O1	176.6 (4)	N2—C3—C6—O4	-84.7 (5)
Cu1—O2—C1—C2	-4.1 (5)	C2—C3—C6—O4	92.9 (5)
C5—N1—C2—C3	-1.6 (6)	N2—C3—C6—O3	90.7 (4)
Cu1—N1—C2—C3	177.6 (3)	C2—C3—C6—O3	-91.7 (5)
C5—N1—C2—C1	178.7 (4)	Cu1—O5—C7—N3	179.4 (4)
Cu1—N1—C2—C1	-2.1 (4)	C9—N3—C7—O5	0.6 (9)
O1—C1—C2—N1	-176.6 (4)	C8—N3—C7—O5	179.3 (6)
O2—C1—C2—N1	4.1 (5)		

Symmetry codes: (i) $-x+1, y-1/2, -z+1/2$; (ii) $x, -y+3/2, z-1/2$; (iii) $-x+1, y+1/2, -z+1/2$; (iv) $x, -y+3/2, z+1/2$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O6—H6B \cdots O4 ^v	0.82 (5)	2.00 (3)	2.771 (5)	156 (7)
O6—H6A \cdots O1 ^{vi}	0.82 (5)	2.38 (3)	3.138 (6)	153 (5)
O6—H6A \cdots O2 ^{vi}	0.82 (5)	2.30 (3)	3.037 (5)	149 (5)

Symmetry codes: (v) $x, y-1, z$; (vi) $-x+1, -y+1, -z$.

Fig. 1

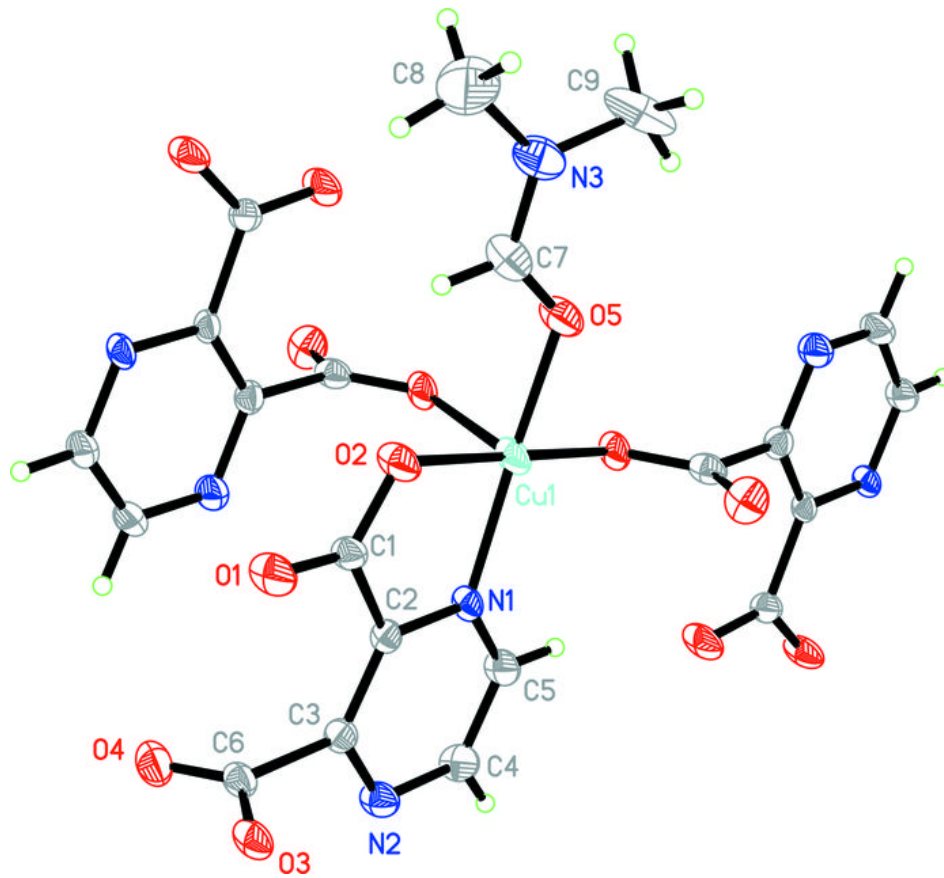


Fig. 2

