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catena-Poly[[aqua(pyrazine-2-carboxylato)copper(II)]-μ-pyrazine-2-carboxylato]

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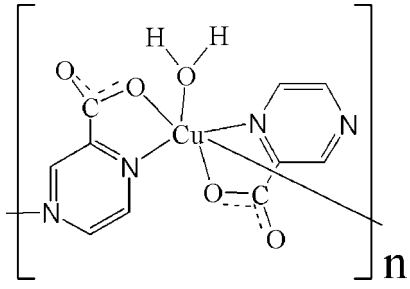
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.038; wR factor = 0.099; data-to-parameter ratio = 13.5.

The title compound, $[Cu(C_5H_3N_2O_2)_2(H_2O)]_n$, prepared by hydrothermal synthesis, is isostructural with its Fe^{II}-, Co^{II}- and Ni^{II}-containing analogues. The asymmetric unit contains two bidendate pyrazine-2-carboxylate (pc) anions bonded to Cu in the equatorial plane through one N and one O atom. The Cu atoms are linked into chains by the second N atom of one of the pc anions bonding to an axial site of a neighbouring Cu atom. The slightly distorted octahedral coordination around Cu is completed by a water molecule, which forms hydrogen bonds to link the chains into a three-dimensional structure. The crystal studied was an inversion twin.

Related literature

For the isostructural Fe^{II}, Co^{II}, and Ni^{II} analogues, see: Hao & Liu (2007); Hao *et al.* (2007); Gao *et al.* (2007).



Experimental

Crystal data

$[Cu(C_5H_3N_2O_2)_2(H_2O)]$
M_r = 327.74
Orthorhombic, $P2_12_12_1$
a = 7.7379 (5) Å
b = 9.9021 (5) Å
c = 15.002 (1) Å
V = 1149.48 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.93 mm^{-1}
T = 298 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: none
6840 measured reflections
2460 independent reflections
2219 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.099
S = 1.01
2460 reflections
182 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Absolute structure: Flack (1983), with 1004 Friedel pairs
Flack parameter: 0.49 (2)

Table 1
Selected bond lengths (Å).

Cu1—O1	2.015 (3)	Cu1—N3	2.089 (3)
Cu1—O3	2.023 (3)	Cu1—N1	2.099 (3)
Cu1—O5	2.073 (3)	Cu1—N2^{i}	2.137 (3)

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H2W···O3^{ii}	0.82 (5)	1.86 (5)	2.682 (4)	177 (7)
O5—H1W···O1^{iii}	0.82 (5)	2.01 (4)	2.757 (4)	153 (7)

Symmetry codes: (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$.

Data collection: *APEX2* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); 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: HB2444).

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supplementary materials

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catena-Poly[[aqua(pyrazine-2-carboxylato)copper(II)]-μ-pyrazine-2-carboxylato]

Y.-X. Gao, L.-B. Wang, Y.-L. Niu and L.-J. Hao

Comment

The title compound, (I), is isostructural with its Fe^{II}, Co^{II}, and Ni^{II} analogues [Hao & Liu, (2007); Hao, Mu & Liu, (2007); Gao *et al.* (2007)]. The Cu^{II} atom in (I) is coordinated in a bidentate fashion by two O and two N atoms from two independent pyrazine-2-carboxylate anions. The distorted octhedral coordiantion is completed by another N atom from a third pyrazine-2-carboxylate ligand, and by the O atom of a water molecule (Fig. 1, Table 1). One pyrazine-2-carboxylate ligand coordinates to a neighboring Cu atom *via* its second N atom, leading to a polymeic structure with zigzag chains extending parallel to the *b* axis (Fig. 2). Hydrogen bonding involving the water molecules (Table 2) stablizes the structure.

Experimental

A mixture of copper dichloride hexahydrate (0.5 mmol), potassium hydroxide (0.5 mmol), 2-pyrazine caboxylic acid (0.5 mmol), EtOH (8 ml) and H_2O (8 ml) in a 25 ml Teflon-lined stainless steel autoclave was heated to at 413 K for 2 d, and then cooled to room temperature. Red block-shaped crystals of (I) were obtained in a yield of 36%. Anal. Calc. for $C_{10}H_8CuN_4O_5$: C 36.62, H 2.44, N 17.09%; Found: C 36.59, H 2.47, N 17.01%.

Refinement

All H atoms on C atoms were generated geometrically (C—H = 0.93 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms of the water molecule were located from difference density maps and were refined with distance restraints of O—H = 0.82 (1) Å and H···H = 1.38 (2) Å and a fixed $U_{iso}(H)$ of 0.08 $Å^2$.

Figures

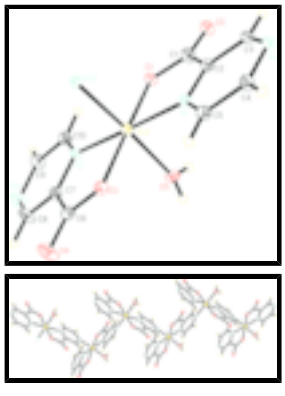

Fig. 1. A fragment of the structure of (I) showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms). Atoms labeled with I at the symmetry positions ($-x + 1$, $y - 1/2$, $-z + 3/2$).

catena-Poly[[aqua(pyrazine-2-carboxylato)copper(II)]-μ-pyrazine-2-carboxylato]

Crystal data

$[Cu(C_5H_3N_2O_2)_2(H_2O)]$	$F_{000} = 660$
$M_r = 327.74$	$D_x = 1.894$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 2460 reflections
$a = 7.7379$ (5) Å	$\theta = 2.5$–27.0º
$b = 9.9021$ (5) Å	$\mu = 1.93$ mm^{-1}
$c = 15.002$ (1) Å	$T = 298$ (2) K
$V = 1149.48$ (12) Å^3	Cube, blue
$Z = 4$	0.10 × 0.10 × 0.10 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	2219 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.032$
Monochromator: graphite	$\theta_{max} = 27.0$º
$T = 298(2)$ K	$\theta_{min} = 2.5$º
φ and ω scans	$h = -8\rightarrow9$
Absorption correction: none	$k = -12\rightarrow12$
6840 measured reflections	$l = -15\rightarrow19$
2460 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.038$	$w = 1/[\sigma^2(F_o^2) + (0.0666P)^2 + 0.3756P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.099$	$(\Delta/\sigma)_{max} = 0.014$
$S = 1.01$	$\Delta\rho_{max} = 1.20$ e Å^{-3}
2460 reflections	$\Delta\rho_{min} = -0.36$ e Å^{-3}
182 parameters	Extinction correction: none
3 restraints	Absolute structure: Flack (1983), with 1004 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.49 (2)
Secondary atom site location: difference Fourier map	

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}
Cu1	0.42685 (6)	0.63422 (4)	0.59076 (3)	0.01911 (14)
C1	0.1940 (5)	0.8096 (4)	0.6830 (3)	0.0259 (5)
C2	0.3720 (5)	0.8540 (4)	0.7110 (2)	0.0174 (7)
C3	0.3948 (5)	0.9581 (4)	0.7733 (3)	0.0214 (8)
H3	0.2981	1.0026	0.7955	0.026*
C4	0.6843 (6)	0.9334 (4)	0.7638 (3)	0.0243 (9)
H4	0.7954	0.9589	0.7804	0.029*
C5	0.6628 (5)	0.8307 (4)	0.6996 (3)	0.0226 (9)
H5	0.7594	0.7905	0.6740	0.027*
C6	0.6424 (6)	0.4713 (4)	0.4810 (3)	0.0228 (9)
C7	0.4616 (5)	0.4269 (4)	0.4590 (3)	0.0232 (9)
C8	0.4259 (6)	0.3353 (4)	0.3918 (3)	0.0323 (10)
H8	0.5175	0.2988	0.3597	0.039*
C9	0.1408 (6)	0.3514 (4)	0.4213 (3)	0.0307 (9)
H9	0.0268	0.3269	0.4101	0.037*
C10	0.1755 (6)	0.4432 (4)	0.4894 (3)	0.0271 (9)
H10	0.0847	0.4779	0.5230	0.033*
N1	0.5062 (4)	0.7910 (3)	0.6756 (2)	0.0195 (7)
N2	0.5494 (4)	0.9948 (3)	0.8012 (2)	0.0191 (7)
N3	0.3352 (4)	0.4817 (3)	0.5070 (2)	0.0197 (7)
N4	0.2667 (5)	0.2974 (4)	0.3713 (3)	0.0383 (10)
O1	0.1945 (3)	0.7028 (3)	0.63112 (18)	0.0201 (6)
O2	0.0686 (3)	0.8697 (3)	0.70894 (18)	0.0259 (5)
O3	0.6530 (4)	0.5644 (3)	0.54124 (19)	0.0218 (6)
O4	0.7633 (4)	0.4208 (4)	0.4411 (3)	0.0434 (9)
O5	0.4184 (4)	0.7653 (3)	0.48314 (19)	0.0274 (6)
H1W	0.509 (5)	0.793 (6)	0.462 (5)	0.080*
H2W	0.335 (5)	0.815 (6)	0.475 (5)	0.080*

Atomic displacement parameters (Å^2)

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

Cu1	0.0166 (2)	0.0202 (2)	0.0205 (2)	−0.00007 (19)	−0.00077 (19)	−0.00039 (19)
C1	0.0155 (10)	0.0306 (12)	0.0314 (12)	0.0031 (11)	−0.0021 (9)	−0.0043 (10)
C2	0.0168 (17)	0.0186 (17)	0.0168 (17)	0.0012 (14)	−0.0034 (13)	0.0012 (15)
C3	0.021 (2)	0.0237 (18)	0.0189 (18)	0.0014 (15)	0.0012 (16)	−0.0043 (15)
C4	0.019 (2)	0.0229 (19)	0.031 (2)	−0.0010 (17)	−0.0004 (17)	−0.0052 (17)
C5	0.0156 (19)	0.024 (2)	0.029 (2)	0.0018 (16)	0.0015 (16)	−0.0003 (16)
C6	0.0189 (19)	0.024 (2)	0.025 (2)	−0.0033 (16)	0.0005 (16)	0.0005 (16)
C7	0.024 (2)	0.0222 (19)	0.023 (2)	0.0035 (16)	0.0005 (16)	0.0005 (16)
C8	0.023 (2)	0.037 (2)	0.038 (3)	0.003 (2)	0.002 (2)	−0.0162 (17)
C9	0.0215 (19)	0.033 (2)	0.038 (2)	−0.0013 (18)	−0.0046 (18)	−0.007 (2)
C10	0.022 (2)	0.027 (2)	0.032 (2)	0.0010 (17)	0.0026 (18)	−0.0019 (17)
N1	0.0169 (15)	0.0205 (16)	0.0211 (17)	0.0013 (13)	−0.0001 (13)	0.0009 (13)
N2	0.0184 (17)	0.0182 (14)	0.0206 (15)	0.0002 (14)	0.0006 (13)	−0.0037 (12)
N3	0.0185 (16)	0.0182 (16)	0.0223 (16)	0.0007 (13)	−0.0003 (14)	−0.0014 (13)
N4	0.031 (2)	0.041 (2)	0.043 (2)	−0.0074 (18)	−0.0033 (18)	−0.0200 (19)
O1	0.0146 (13)	0.0238 (13)	0.0219 (14)	0.0003 (11)	−0.0022 (11)	−0.0039 (11)
O2	0.0155 (10)	0.0306 (12)	0.0314 (12)	0.0031 (11)	−0.0021 (9)	−0.0043 (10)
O3	0.0135 (13)	0.0233 (14)	0.0286 (15)	−0.0016 (11)	0.0001 (11)	−0.0007 (12)
O4	0.0217 (17)	0.054 (2)	0.054 (2)	0.0074 (16)	0.0067 (15)	−0.0191 (17)
O5	0.0234 (15)	0.0304 (15)	0.0285 (14)	0.0089 (15)	0.0052 (14)	0.0127 (12)

Geometric parameters (Å, °)

Cu1—O1	2.015 (3)	C5—H5	0.9300
Cu1—O3	2.023 (3)	C6—O4	1.218 (5)
Cu1—O5	2.073 (3)	C6—O3	1.293 (5)
Cu1—N3	2.089 (3)	C6—C7	1.503 (6)
Cu1—N1	2.099 (3)	C7—N3	1.331 (5)
Cu1—N2^{i}	2.137 (3)	C7—C8	1.384 (6)
C1—O2	1.203 (5)	C8—N4	1.324 (6)
C1—O1	1.313 (5)	C8—H8	0.9300
C1—C2	1.506 (5)	C9—N4	1.341 (6)
C2—N1	1.323 (5)	C9—C10	1.394 (6)
C2—C3	1.402 (5)	C9—H9	0.9300
C3—N2	1.319 (5)	C10—N3	1.320 (6)
C3—H3	0.9300	C10—H10	0.9300
C4—N2	1.332 (5)	N2—Cu1^{ii}	2.137 (3)
C4—C5	1.410 (6)	O5—H1W	0.82 (5)
C4—H4	0.9300	O5—H2W	0.82 (5)
C5—N1	1.324 (5)		
O1—Cu1—O3	175.85 (12)	O4—C6—O3	126.0 (4)
O1—Cu1—O5	89.69 (12)	O4—C6—C7	119.1 (4)
O3—Cu1—O5	87.45 (12)	O3—C6—C7	114.9 (3)
O1—Cu1—N3	96.98 (12)	N3—C7—C8	121.0 (4)
O3—Cu1—N3	79.95 (12)	N3—C7—C6	116.5 (3)
O5—Cu1—N3	88.47 (13)	C8—C7—C6	122.6 (4)
O1—Cu1—N1	80.18 (12)	N4—C8—C7	122.8 (4)
O3—Cu1—N1	102.86 (13)	N4—C8—H8	118.6

O5—Cu1—N1	91.06 (13)	C7—C8—H8	118.6
N3—Cu1—N1	177.12 (14)	N4—C9—C10	122.0 (4)
O1—Cu1—N2^{i}	93.83 (12)	N4—C9—H9	119.0
O3—Cu1—N2^{i}	89.04 (12)	C10—C9—H9	119.0
O5—Cu1—N2^{i}	176.48 (14)	N3—C10—C9	121.0 (4)
N3—Cu1—N2^{i}	91.07 (13)	N3—C10—H10	119.5
N1—Cu1—N2^{i}	89.57 (12)	C9—C10—H10	119.5
O2—C1—O1	126.3 (4)	C2—N1—C5	118.0 (3)
O2—C1—C2	120.2 (4)	C2—N1—Cu1	111.3 (3)
O1—C1—C2	113.5 (3)	C5—N1—Cu1	130.7 (3)
N1—C2—C3	121.0 (3)	C3—N2—C4	116.8 (3)
N1—C2—C1	117.9 (3)	C3—N2—Cu1^{ii}	119.8 (3)
C3—C2—C1	121.1 (3)	C4—N2—Cu1^{ii}	123.2 (3)
N2—C3—C2	121.9 (4)	C10—N3—C7	117.5 (3)
N2—C3—H3	119.1	C10—N3—Cu1	130.3 (3)
C2—C3—H3	119.1	C7—N3—Cu1	111.8 (3)
N2—C4—C5	121.6 (4)	C9—N4—C8	115.7 (4)
N2—C4—H4	119.2	C1—O1—Cu1	116.9 (2)
C5—C4—H4	119.2	C6—O3—Cu1	116.5 (3)
N1—C5—C4	120.5 (4)	Cu1—O5—H1W	119 (5)
N1—C5—H5	119.8	Cu1—O5—H2W	121 (5)
C4—C5—H5	119.8	H1W—O5—H2W	114 (3)
O2—C1—C2—N1	−175.2 (4)	C5—C4—N2—Cu1^{ii}	172.6 (3)
O1—C1—C2—N1	5.7 (5)	C9—C10—N3—C7	−1.8 (6)
O2—C1—C2—C3	5.3 (6)	C9—C10—N3—Cu1	170.6 (3)
O1—C1—C2—C3	−173.8 (3)	C8—C7—N3—C10	1.5 (6)
N1—C2—C3—N2	−2.1 (6)	C6—C7—N3—C10	−179.4 (4)
C1—C2—C3—N2	177.3 (4)	C8—C7—N3—Cu1	−172.3 (3)
N2—C4—C5—N1	−1.0 (6)	C6—C7—N3—Cu1	6.8 (4)
O4—C6—C7—N3	177.6 (4)	O1—Cu1—N3—C10	−1.5 (4)
O3—C6—C7—N3	−3.8 (5)	O3—Cu1—N3—C10	−178.6 (4)
O4—C6—C7—C8	−3.3 (6)	O5—Cu1—N3—C10	−91.0 (4)
O3—C6—C7—C8	175.3 (4)	N2^{i}—Cu1—N3—C10	92.5 (4)
N3—C7—C8—N4	0.1 (7)	O1—Cu1—N3—C7	171.3 (3)
C6—C7—C8—N4	−179.0 (4)	O3—Cu1—N3—C7	−5.9 (2)
N4—C9—C10—N3	0.6 (7)	O5—Cu1—N3—C7	81.8 (3)
C3—C2—N1—C5	−1.1 (6)	N2^{i}—Cu1—N3—C7	−94.7 (3)
C1—C2—N1—C5	179.4 (4)	C10—C9—N4—C8	1.0 (7)
C3—C2—N1—Cu1	176.9 (3)	C7—C8—N4—C9	−1.3 (7)
C1—C2—N1—Cu1	−2.6 (4)	O2—C1—O1—Cu1	175.0 (4)
C4—C5—N1—C2	2.6 (6)	C2—C1—O1—Cu1	−6.0 (5)
C4—C5—N1—Cu1	−175.0 (3)	O3—Cu1—O1—C1	−133.6 (16)
O1—Cu1—N1—C2	−0.4 (2)	O5—Cu1—O1—C1	−87.4 (3)
O3—Cu1—N1—C2	176.7 (3)	N3—Cu1—O1—C1	−175.8 (3)
O5—Cu1—N1—C2	89.1 (3)	N1—Cu1—O1—C1	3.8 (3)
N2^{i}—Cu1—N1—C2	−94.4 (3)	N2^{i}—Cu1—O1—C1	92.7 (3)

O1—Cu1—N1—C5	177.3 (4)	O4—C6—O3—Cu1	177.0 (4)
O3—Cu1—N1—C5	−5.6 (4)	C7—C6—O3—Cu1	−1.6 (4)
O5—Cu1—N1—C5	−93.2 (4)	O1—Cu1—O3—C6	−38.5 (18)
N2^{i}—Cu1—N1—C5	83.3 (4)	O5—Cu1—O3—C6	−84.9 (3)
C2—C3—N2—C4	3.7 (6)	N3—Cu1—O3—C6	4.0 (3)
C2—C3—N2—Cu1^{ii}	−171.3 (3)	N1—Cu1—O3—C6	−175.4 (3)
C5—C4—N2—C3	−2.2 (6)	N2^{i}—Cu1—O3—C6	95.3 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H2W···O3^{iii}	0.82 (5)	1.86 (5)	2.682 (4)	177 (7)
O5—H1W···O1^{iv}	0.82 (5)	2.01 (4)	2.757 (4)	153 (7)

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

Fig. 1

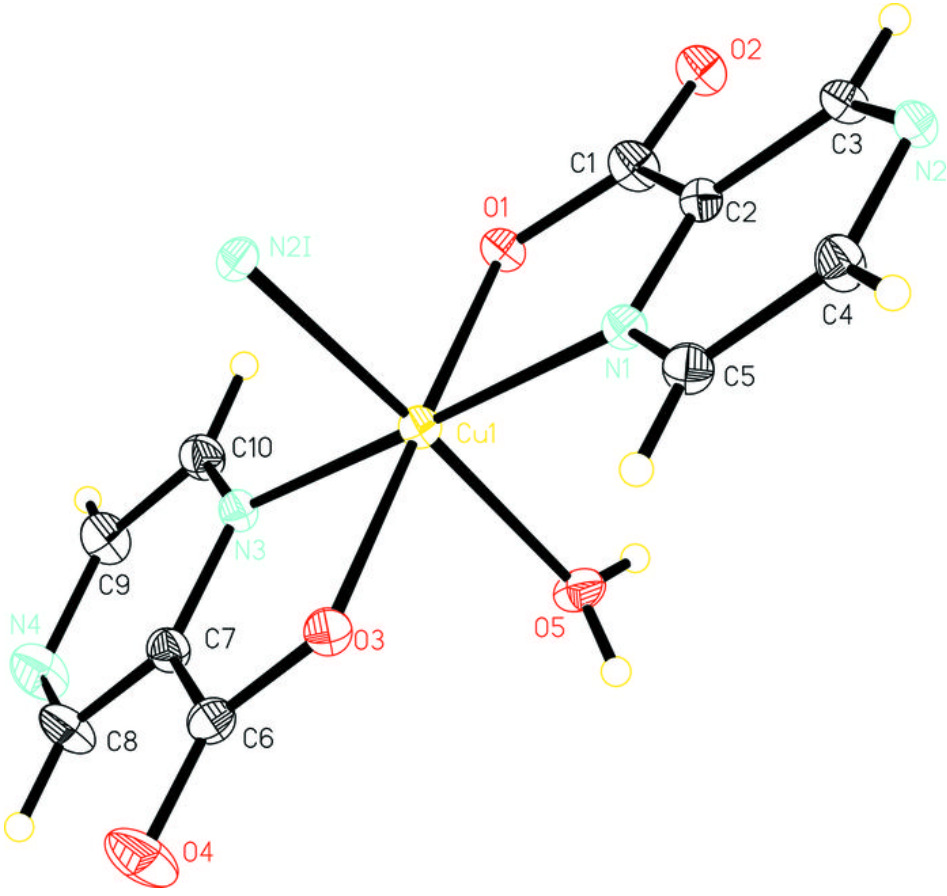

Fig. 2