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(4-Aminobenzoato-κ^2O,O')chlorido-(di-2-pyridylamine-κ^2N,N')copper(II) monohydrate

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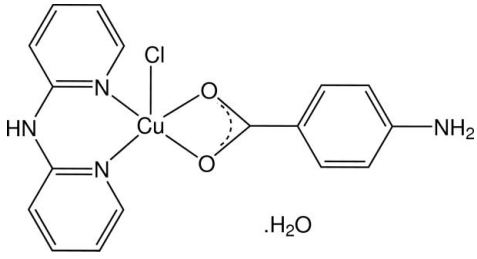
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.002 Å; R factor = 0.021; wR factor = 0.062; data-to-parameter ratio = 16.2.

In the title compound, $[Cu(C_7H_6NO_2)Cl(C_{10}H_9N_3)]\cdot H_2O$, the Cu atom has a distorted square-pyramidal geometry defined by one *N*,*N*-bidentate 2,2′-bipyridylamine ($C_{10}H_9N_3$) molecule, one *O*,*O*-bidentate *p*-aminobenzenecarboxylate ($C_7H_6NO_2^-$) anion and one apical chlorido ligand. The Cu atom deviates from the mean plane of the basal atoms towards the Cl atom by 0.2591 (1) Å. The component species are connected to each other by N—H···Cl, O—H···Cl, N—H···O and O—H···O hydrogen bonds.

Related literature

For related literature, see: Brophy *et al.* (1999); Mao *et al.* (2004); Okabe *et al.* (2007); Wang & Okabe (2005); Yodoshi, Mototsuji & Okabe (2007); Yodoshi, Odoko & Okabe (2007); Youngme *et al.* (2004).



Experimental

Crystal data

$[Cu(C_7H_6NO_2)Cl(C_{10}H_9N_3)]\cdot H_2O$
M_r = 424.35
Monoclinic, $P2_1/n$
a = 9.86 (1) Å
b = 12.10 (1) Å
c = 14.60 (1) Å
β = 100.63 (3)°
V = 1712 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.46 mm^{-1}
T = 123.1 K
0.30 × 0.30 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.728, T_{max} = 0.851
16167 measured reflections
3922 independent reflections
3424 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.062
S = 1.07
3922 reflections
242 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—Cl1	2.596 (3)	Cu1—N1	1.948 (1)
Cu1—O1	2.080 (1)	Cu1—N2	1.973 (1)
Cu1—O2	1.972 (1)		
O1—Cu1—O2	64.96 (4)	N1—Cu1—N2	93.69 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H9···Cl1^{i}	0.86	2.35	3.196 (3)	169
N4—H14···O3^{ii}	0.86	2.11	2.968 (2)	174
N4—H15···Cl1^{iii}	0.86	2.71	3.547 (2)	166
O3—H16···Cl1	0.82	2.47	3.263 (4)	164
O3—H17···O1^{iv}	0.80	2.13	2.911 (2)	166

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2005) and *CRYSTALS* (Betteridge *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997), and *PLATON* (Spek, 2003); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2471).

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supplementary materials

Acta Cryst. (2007). E**63**, m2108-m2109 [**doi:10.1107/S1600536807032837**]

(4-Aminobenzoato-κ^2O,O')chlorido(di-2-pyridylamine-κ^2N,N')copper(II) monohydrate

N. Okabe, A. Tsuji and M. Yodoshi

Comment

As part of our studies of new therapeutic drugs, we have reported the structures of the ternary Cu(II) complexes with the heterocyclic ligand, 2,2'-bipyridylamine (bpa) and various carboxylate-containing compounds, such as bpa and *p*-hydroxybenzenecarboxylate (*p*-HB) (Wang & Okabe, 2005), cyclobutane-1,1-dicarboxylate (Yodoshi, Mototsuji & Okabe, 2007), benzenecarboxylate (BA) (Okabe *et al.*, 2007), and glycine (Yodoshi, Odoko & Okabe, 2007). In this study, we report the structure of the title Cu(II) complex, (I), with bpa and the *p*-aminobenzenecarboxylate (*p*-ABA) and chloride anions. An uncoordinated water molecule completes the structure.

The overall structure of (I) is similar to those of the Cu(II) complexes with bpa and *p*-HB (Wang & Okabe, 2005) and BA (Okabe *et al.*, 2007). The central Cu atom in (I) (Fig. 1) has a square pyramidal CuN_2O_2Cl geometry (Table 1), resulting from its coordination by two N atoms from one bpa and two O atoms from one *p*-ABA and one chloride anion. The four basal ligand atoms (N1, N2,O1 and O2) are neary coplanar, and the Cu atom deviates from the mean square plane towards the apical Cl atom by 0.2591 (1) Å. The bite angles N1—Cu1—N2 and O1—Cu1—O2 are in the range normally observed for these complexes (Wang & Okabe, 2005; Okabe *et al.*, 2007; Yodoshi, Mototsuji & Okabe, 2007; Yodoshi, Odoko & Okabe, 2007; Youngme *et al.*, 2004). The Cu—Cl distance of 2.597 (1)%A in (I) is slightly longer than the median of the known values from 2.336 (2) to 2.733 (2) Å (Mao *et al.*, 2004; Brophy *et al.*, 1999) Such long Cu—Cl bonds are explained by the well known Jahn-Teller effect.

As shown in Fig. 2, the crystal structure of (I) is stabilized by N—H···Cl, O—H···Cl, N—H···O, and O—H···O hydrogen bonds (Table 2), and no π-π stacking interactions are present.

Experimental

2,2'-Bipyridylamine (5.0 mg, 0.03 mol) dissolved in 90%(*v*/*v*) methanol-water solution (2 ml) was reacted with *p*-aminobenzoic acid (4.0 mg, 0.03 mol), dissolved in the same solution (2 ml) for 5 min at room temperature. This was followed by the addition of $CuCl_2{\cdot}2H_2O$ (5.0 mg, 0.03 mol) dissolved in H_2O (1 ml) and reacted for 15 min at room temperature. After several days green prismatic crystals of (I) appeared from the mother liquor.

Refinement

The water H atoms were located in a difference map and refined as riding in their as-found relative postions with U_{iso}(H) = 1.5U_{eq}(O). The C– and N-bound H atoms were located in difference maps, relocated in idealized positions and treated as riding, with C—H = 0.93 Å, N—H = 0.86Å and U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

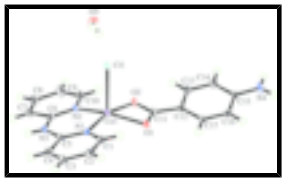

Fig. 1. View of the molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level (arbitrary spheres for the H atoms).

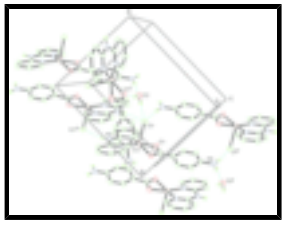

Fig. 2. A view of the hydrogen bonds (dashed lines) in (I). Symmetry codes as in Table 2.

(4-Aminobenzoato-κ^2*O*,*O*')chlorido(di-2-pyridylamine-\ κ^2*N*,*N*')copper(II) monohydrat

Crystal data

$[Cu(C_7H_6NO_2)Cl(C_{10}H_9N_3)]\cdot H_2O$	F_{000} = 868.00
M_r = 424.35	D_x = 1.646 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.7107 Å
Hall symbol: -P 2yn	Cell parameters from 14678 reflections
a = 9.86 (1) Å	θ = 3.2–27.5º
b = 12.10 (1) Å	μ = 1.46 mm^{-1}
c = 14.60 (1) Å	T = 123.1 K
β = 100.63 (3)º	Prism, green
V = 1712 (3) Å^3	0.30 × 0.30 × 0.10 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	3424 reflections with $F^2 > 2.0\sigma(F^2)$
Detector resolution: 10.00 pixels mm^{-1}	R_{int} = 0.017
ω scans	θ_{max} = 27.5º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	h = −12→12
T_{min} = 0.728, T_{max} = 0.851	k = −14→15
16167 measured reflections	l = −18→18
3922 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.021	$w = 1/[\sigma^2(F_o^2) + (0.036P)^2 + 0.6204P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.062$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.07$	$\Delta\rho_{max} = 0.36$ e Å^{-3}
3922 reflections	$\Delta\rho_{min} = -0.42$ e Å^{-3}
242 parameters	Extinction correction: none

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (S) are based on F^2. *R*-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating *R*-factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.93181 (2)	0.23066 (1)	0.48560 (1)	0.01293 (6)
Cl1	0.70895 (4)	0.33281 (3)	0.40723 (2)	0.01702 (8)
O1	0.9042 (1)	0.08460 (8)	0.40938 (7)	0.0156 (2)
O2	0.8285 (1)	0.11464 (8)	0.53813 (7)	0.0177 (2)
O3	0.5317 (1)	0.51357 (9)	0.26822 (8)	0.0225 (2)
N1	1.0627 (1)	0.3078 (1)	0.42339 (8)	0.0131 (2)
N2	0.9776 (1)	0.32012 (9)	0.60007 (8)	0.0137 (2)
N3	1.1401 (1)	0.43479 (9)	0.54583 (8)	0.0140 (2)
N4	0.4964 (1)	−0.3283 (1)	0.41741 (9)	0.0212 (3)
C1	1.0691 (1)	0.2727 (1)	0.3360 (1)	0.0160 (3)
C2	1.1551 (1)	0.3188 (1)	0.2827 (1)	0.0178 (3)
C3	1.2434 (1)	0.4038 (1)	0.3211 (1)	0.0185 (3)
C4	1.2391 (1)	0.4396 (1)	0.4095 (1)	0.0169 (3)
C5	1.1449 (1)	0.3914 (1)	0.45928 (9)	0.0129 (2)
C6	1.0676 (1)	0.4034 (1)	0.61365 (9)	0.0128 (2)
C7	1.0937 (1)	0.4632 (1)	0.69802 (9)	0.0162 (3)
C8	1.0244 (2)	0.4345 (1)	0.7678 (1)	0.0196 (3)
C9	0.9302 (2)	0.3477 (1)	0.7538 (1)	0.0221 (3)
C10	0.9100 (2)	0.2933 (1)	0.6701 (1)	0.0189 (3)
C11	0.8334 (1)	0.0513 (1)	0.46906 (9)	0.0137 (3)
C12	0.7553 (1)	−0.0525 (1)	0.45855 (9)	0.0131 (3)
C13	0.6597 (1)	−0.0730 (1)	0.51656 (9)	0.0159 (3)
C14	0.5743 (1)	−0.1639 (1)	0.50303 (9)	0.0170 (3)
C15	0.5830 (1)	−0.2395 (1)	0.4310 (1)	0.0151 (3)
C16	0.6805 (1)	−0.2201 (1)	0.37370 (9)	0.0141 (3)
C17	0.7645 (1)	−0.1280 (1)	0.38739 (9)	0.0138 (3)
H1	1.0125	0.2146	0.3110	0.019*
H2	1.1545	0.2941	0.2223	0.021*
H3	1.3044	0.4356	0.2871	0.022*
H4	1.2981	0.4954	0.4364	0.020*
H5	1.1568	0.5211	0.7062	0.019*
H6	1.0402	0.4728	0.8239	0.024*

H7	0.8822	0.3271	0.8002	0.027*
H8	0.8471	0.2353	0.6607	0.023*
H9	1.1917	0.4918	0.5601	0.017*
H10	0.6539	−0.0245	0.5650	0.019*
H11	0.5105	−0.1754	0.5417	0.020*
H12	0.6884	−0.2696	0.3263	0.017*
H13	0.8282	−0.1159	0.3487	0.017*
H14	0.5007	−0.3740	0.3729	0.025*
H15	0.4376	−0.3386	0.4533	0.025*
H16	0.5769	0.4615	0.2935	0.034*
H17	0.5563	0.5234	0.2197	0.034*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0154 (1)	0.0118 (1)	0.0125 (1)	−0.00460 (6)	0.00479 (6)	−0.00184 (5)
Cl1	0.0150 (2)	0.0150 (2)	0.0205 (2)	−0.0028 (1)	0.0018 (1)	0.0013 (1)
O1	0.0181 (5)	0.0133 (5)	0.0165 (5)	−0.0038 (4)	0.0061 (4)	−0.0009 (3)
O2	0.0236 (6)	0.0142 (5)	0.0165 (5)	−0.0071 (4)	0.0071 (4)	−0.0031 (4)
O3	0.0275 (6)	0.0224 (6)	0.0199 (6)	0.0061 (5)	0.0103 (4)	0.0033 (4)
N1	0.0128 (6)	0.0132 (6)	0.0135 (5)	−0.0009 (4)	0.0033 (4)	0.0000 (4)
N2	0.0147 (6)	0.0139 (6)	0.0126 (5)	−0.0023 (4)	0.0029 (4)	−0.0006 (4)
N3	0.0149 (6)	0.0122 (6)	0.0151 (6)	−0.0055 (4)	0.0034 (4)	−0.0019 (4)
N4	0.0250 (7)	0.0188 (6)	0.0210 (6)	−0.0108 (5)	0.0078 (5)	−0.0044 (5)
C1	0.0156 (7)	0.0163 (7)	0.0163 (7)	−0.0020 (5)	0.0032 (5)	−0.0028 (5)
C2	0.0184 (7)	0.0213 (7)	0.0150 (7)	−0.0001 (6)	0.0063 (5)	−0.0019 (5)
C3	0.0158 (7)	0.0218 (7)	0.0198 (7)	−0.0023 (6)	0.0079 (5)	0.0018 (5)
C4	0.0141 (7)	0.0171 (7)	0.0198 (7)	−0.0045 (5)	0.0039 (5)	−0.0001 (5)
C5	0.0121 (6)	0.0136 (6)	0.0131 (6)	0.0006 (5)	0.0022 (5)	0.0010 (5)
C6	0.0116 (6)	0.0126 (6)	0.0137 (6)	0.0010 (5)	0.0011 (5)	0.0006 (5)
C7	0.0150 (7)	0.0169 (7)	0.0163 (7)	−0.0038 (5)	0.0012 (5)	−0.0031 (5)
C8	0.0212 (8)	0.0243 (8)	0.0128 (7)	−0.0043 (6)	0.0021 (5)	−0.0049 (5)
C9	0.0258 (8)	0.0279 (8)	0.0141 (7)	−0.0094 (6)	0.0077 (6)	−0.0025 (6)
C10	0.0213 (8)	0.0198 (7)	0.0168 (7)	−0.0073 (6)	0.0066 (5)	−0.0022 (5)
C11	0.0132 (7)	0.0130 (6)	0.0142 (6)	0.0002 (5)	0.0008 (5)	0.0013 (5)
C12	0.0139 (7)	0.0111 (6)	0.0137 (6)	−0.0012 (5)	0.0008 (5)	0.0015 (4)
C13	0.0199 (7)	0.0149 (7)	0.0133 (6)	−0.0020 (5)	0.0041 (5)	−0.0012 (5)
C14	0.0192 (7)	0.0180 (7)	0.0150 (7)	−0.0041 (5)	0.0061 (5)	0.0001 (5)
C15	0.0159 (7)	0.0133 (6)	0.0149 (7)	−0.0019 (5)	−0.0003 (5)	0.0019 (5)
C16	0.0157 (7)	0.0133 (7)	0.0127 (6)	0.0005 (5)	0.0011 (5)	−0.0007 (4)
C17	0.0136 (7)	0.0144 (6)	0.0134 (6)	0.0020 (5)	0.0025 (5)	0.0027 (5)

Geometric parameters (Å, °)

Cu1—Cl1	2.596 (3)	C3—C4	1.370 (2)
Cu1—O1	2.080 (1)	C3—H3	0.9300
Cu1—O2	1.972 (1)	C4—C5	1.408 (2)
Cu1—N1	1.948 (1)	C4—H4	0.9300
Cu1—N2	1.973 (1)	C6—C7	1.411 (2)

O1—C11	1.278 (2)	C7—C8	1.371 (2)
O2—C11	1.275 (2)	C7—H5	0.9299
O3—H16	0.8189	C8—C9	1.393 (2)
O3—H17	0.7997	C8—H6	0.9300
N1—C1	1.358 (2)	C9—C10	1.370 (2)
N1—C5	1.341 (2)	C9—H7	0.9299
N2—C6	1.334 (2)	C10—H8	0.9300
N2—C10	1.359 (2)	C11—C12	1.468 (2)
N3—C5	1.378 (2)	C12—C13	1.401 (2)
N3—C6	1.378 (2)	C12—C17	1.399 (2)
N3—H9	0.8601	C13—C14	1.378 (2)
N4—C15	1.364 (2)	C13—H10	0.9299
N4—H14	0.8600	C14—C15	1.408 (2)
N4—H15	0.8600	C14—H11	0.9299
C1—C2	1.371 (2)	C15—C16	1.406 (2)
C1—H1	0.9300	C16—C17	1.382 (2)
C2—C3	1.397 (2)	C16—H12	0.9299
C2—H2	0.9301	C17—H13	0.9300
O1—Cu1—O2	64.96 (4)	H4—C4—C3	120.1972
O1—Cu1—N1	100.99 (5)	C7—C6—N2	121.8 (1)
O1—Cu1—N2	155.07 (4)	C7—C6—N3	116.8 (1)
O2—Cu1—N1	163.19 (5)	C8—C7—C6	118.9 (1)
O2—Cu1—N2	96.61 (5)	C8—C7—H5	120.5419
N1—Cu1—N2	93.69 (5)	H5—C7—C6	120.5617
C11—O1—Cu1	86.39 (8)	C9—C8—C7	119.5 (1)
C11—O2—Cu1	91.27 (9)	C9—C8—H6	120.2575
H16—O3—H17	106.5428	H6—C8—C7	120.2656
C1—N1—Cu1	116.01 (9)	C10—C9—C8	118.5 (2)
C1—N1—C5	118.2 (1)	C10—C9—H7	120.7387
C5—N1—Cu1	125.8 (1)	H7—C9—C8	120.7571
C6—N2—Cu1	125.6 (1)	H8—C10—N2	118.4789
C6—N2—C10	118.3 (1)	H8—C10—C9	118.4777
C10—N2—Cu1	116.05 (9)	C12—C11—O1	122.7 (1)
C5—N3—C6	131.6 (1)	C12—C11—O2	120.1 (1)
C5—N3—H9	114.1757	C13—C12—C11	119.2 (1)
C6—N3—H9	114.1759	C13—C12—C17	118.5 (1)
C15—N4—H14	120.0009	C17—C12—C11	122.1 (1)
C15—N4—H15	119.9993	C14—C13—C12	121.1 (1)
H14—N4—H15	119.9998	C14—C13—H10	119.4483
C2—C1—N1	123.2 (1)	H10—C13—C12	119.4502
C2—C1—H1	118.3955	C15—C14—C13	120.4 (1)
H1—C1—N1	118.3871	C15—C14—H11	119.8033
C3—C2—C1	118.5 (1)	H11—C14—C13	119.8016
C3—C2—H2	120.7520	C16—C15—N4	121.5 (1)
H2—C2—C1	120.7608	C16—C15—C14	118.6 (1)
C4—C3—C2	119.1 (1)	C17—C16—C15	120.4 (1)
C4—C3—H3	120.4688	C17—C16—H12	119.7788
H3—C3—C2	120.4693	H12—C16—C15	119.7821
C5—C4—C3	119.6 (1)	H13—C17—C12	119.5207

C5—C4—H4	120.2014	H13—C17—C16	119.5239
O2—Cu1—O1—C11	3.07 (6)	C1—C2—C3—C4	−1.4 (2)
O1—Cu1—O2—C11	−3.07 (7)	C2—C3—C4—C5	−0.8 (2)
O1—Cu1—N1—C1	20.2 (1)	C3—C4—C5—N1	2.7 (2)
O1—Cu1—N2—C6	128.1 (1)	C3—C4—C5—N3	−176.6 (1)
Cu1—O1—C11—O2	−4.8 (1)	N2—C6—C7—C8	0.1 (2)
Cu1—O2—C11—O1	5.1 (1)	C6—C7—C8—C9	−0.1 (2)
Cu1—N1—C1—C2	179.5 (1)	C7—C8—C9—C10	0.1 (2)
Cu1—N1—C5—N3	−2.7 (2)	C8—C9—C10—N2	−0.0 (2)
Cu1—N1—C5—C4	178.1 (1)	O1—C11—C12—C13	−167.7 (1)
Cu1—N2—C6—N3	−0.4 (2)	C11—C12—C13—C14	173.4 (1)
Cu1—N2—C10—C9	−179.9 (1)	C11—C12—C17—C16	−173.9 (1)
C6—N3—C5—N1	5.3 (2)	C12—C13—C14—C15	1.0 (2)
C6—N3—C5—C4	−175.5 (1)	C13—C14—C15—N4	−179.0 (1)
C5—N3—C6—N2	−3.6 (2)	N4—C15—C16—C17	178.3 (1)
H14—N4—C15—C14	179.0	C15—C16—C17—C12	0.4 (2)
N1—C1—C2—C3	2.0 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H9···Cl1^{i}	0.86	2.35	3.196 (3)	169
N4—H14···O3^{ii}	0.86	2.11	2.968 (2)	174
N4—H15···Cl1^{iii}	0.86	2.71	3.547 (2)	166
O3—H16···Cl1	0.82	2.47	3.263 (4)	164
O3—H17···O1^{iv}	0.80	2.13	2.911 (2)	166

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

Fig. 1

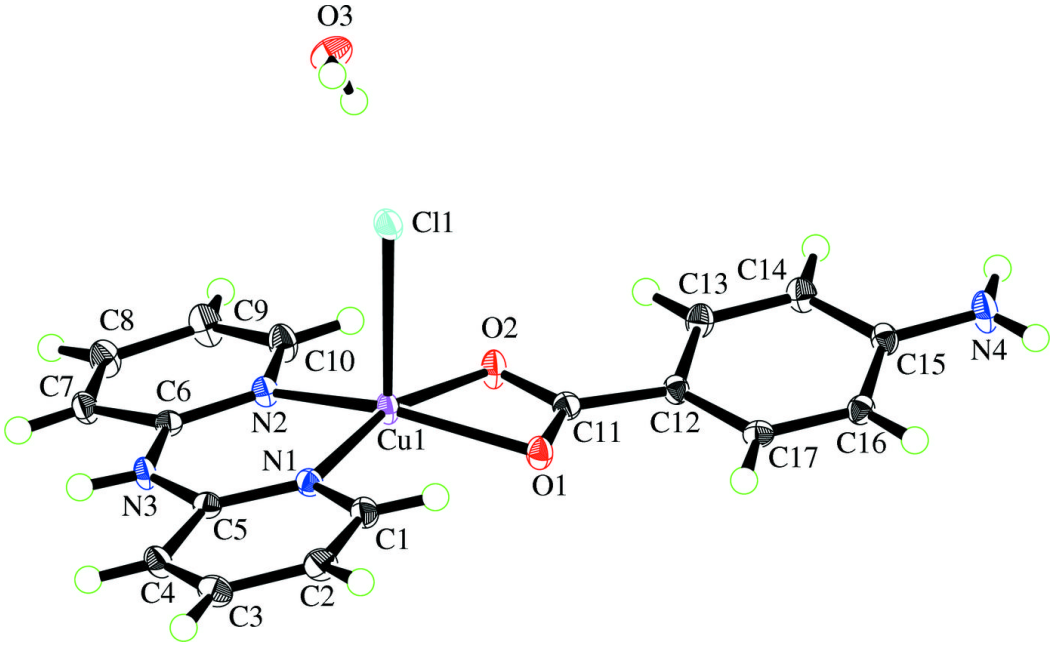
O3
Cl1
C13
C14
C8
C9
O2
C15
N4
C7
C6
C10
N2
Cu1
C11
C12
C17
C16
N1
O1
N3
C5
C1
C4
C2
C3

Fig. 2