Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(Benzoato-κ^2O,O')chlorido(2,9-dimethyl-1,10-phenanthroline-κ^2N,N')-copper(II)

Xiao-Peng Xuan,* Pei-Zheng Zhao and Shu-Xia Zhang

Department of Chemistry, Henan Normal University, Xinxiang 453007, People's Republic of China
Correspondence e-mail: xpxuan@henannu.edu.cn

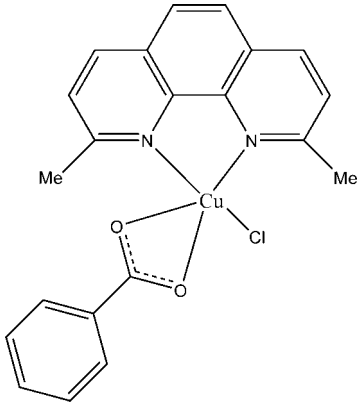
Received 12 May 2007; accepted 31 May 2007

Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; R factor = 0.040; wR factor = 0.118; data-to-parameter ratio = 14.2.

In the title compound, $[Cu(C_7H_5O_2)Cl(C_{14}H_{12}N_2)]$, the Cu^{II} ion is five-coordinated in a distorted square-pyramidal geometry by two O atoms from one benzoate anion, two N atoms from one 2,9-dimethyl-1,10-phenanthroline ligand (dmphen) and one Cl^- anion. The Cu—N bond lengths are 1.990 (3) and 2.111 (3) Å, while the Cu—O bond lengths are 2.031 (2) and 2.069 (2) Å. The crystal packing seems to be determined by interactions between dmphen aromatic rings of neighbouring molecules, with a distance between their ring centroids of 3.978 (5) Å.

Related literature

For related literature, see: Pallenberg *et al.* (1995); Tian & Long (2000); Paulovicova *et al.* (2001); Lemoine *et al.* (2003).



Experimental

Crystal data

$[Cu(C_7H_5O_2)Cl(C_{14}H_{12}N_2)]$
M_r = 428.36
Monoclinic, $P2_1/n$
a = 8.0991 (8) Å
b = 15.9385 (15) Å
c = 15.0440 (14) Å
β = 104.610 (1)°
V = 1879.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.32 mm^{-1}
T = 291 (2) K
0.36 × 0.27 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.634, T_{max} = 0.727
14114 measured reflections
3499 independent reflections
2627 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.118
S = 1.03
3499 reflections
246 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; 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*.

Financial support by the Science Fund of Henan Province for Distinguished Young Scholars (No. 074100510005) is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2106).

References

Bruker (1997). *SMART*, *SAINT*, *SADABS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Lemoine, P., Viossat, B. & Daran, J.-C. (2003). *Acta Cryst.* E**59**, m17–m19.
Pallenberg, A. J., Koenig, K. S. & Barnhart, D. M. (1995). *Inorg. Chem.* **34**, 2833–2840.
Paulovicova, A., El-Ayaan, U. & Fukuda, Y. (2001). *Inorg. Chim. Acta*, **321**, 56–62.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tian, L. & Long, X.-Y. (2000). *Chin. J. Struct. Chem.* **19**, 363–367. (In Chinese.)

 doi:10.1107/S1600536807026773

supplementary materials

Acta Cryst. (2007). E**63**, m1817 [**doi:10.1107/S1600536807026773**]

(Benzoato-κ^2O,O')chlorido(2,9-dimethyl-1,10-phenanthroline-κ^2N,N')copper(II)

X.-P. Xuan, P.-Z. Zhao and S.-X. Zhang

Comment

Copper(II) complexes of 1,10-phenanthroline and its derivatives have attracted much attention because of their peculiar features (Paulovicova *et al.*, 2001; Pallenberg *et al.*, 1995). Recently, we obtained the title mononuclear copper(II) complex, (I), by reaction of copper dichloride, sodium benzoate and 2,9-dimethyl-1,10-phenanthroline (dmphen) in an ethanol/water mixture, and its crystal structure is reported here.

The Cu^{II} ion in (I) has a distorted square-pyramidal geometry, with the apical position occupied by one Cl^- anion (Fig. 1). Two N atoms of one dmphen molecule and two O atoms of one benzoate anion form the basal plane.

Molecules in the crystal are arranged in chains formed by π–π stacking of the dmphen molecules (Fig. 2). These intermolecular interactions occur between rings C8···C11/N1/C13 and C2···C5/C14/N2 within the staggered conformation. The distance between the ring centroids *X*(1 A) and *X*(1B) and the perpendicular distance from *X*(1 A) to *X*(1B) rings (symmetry code for symmetry related molecules: 1 + *x*, 1/2 + *y*, -*z*) are 3.978 (5) and 3.614 (5) Å, respectively. The dihedral angle between these planes is 2.8 (5)°.

Experimental

To a solution of 2,9-dimethyl-1,10-phenanthroline hemihydrate ($C_{14}H_{12}N_2.0.5\ H_2O$, 0.22 g, 1 mmol) and sodium benzoate (0.17 g, 1 mmol) in ethanol/water (20 ml) was added a solution of $CuCl_2{\cdot}2H_2O$ (0.18 g, 1 mmol) in distilled water (10 ml). The resulting solution was refluxed for 1 h and then a pale green precipitate was filtered. Blue single crystals of (I) were obtained by slow evaporation of the filtrate after 1 d.

Refinement

H atoms were positioned geometrically and treated as riding, with C—H distances in the range 0.95–0.99 Å and with U_{iso}(H) = 1.2U_{eq}(C).

Figures

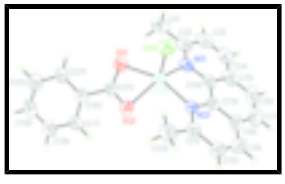


Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

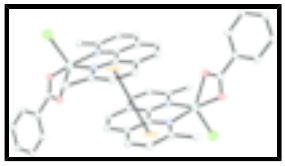


Fig. 2. The π–π interactions between dmphen ligands in the crystal structure of (I). H atoms have been omitted for clarity.

(Benzoato-κ^2*O*,*O*')chlorido(2,9-dimethyl-1,10-phenanthroline- κ^2*N*,*N*')copper(II)

Crystal data

$[Cu(C_7H_5O_2)Cl(C_{14}H_{12}N_2)]$	F_{000} = 876
M_r = 428.36	D_x = 1.514 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 4230 reflections
a = 8.0991 (8) Å	θ = 2.6–22.1º
b = 15.9385 (15) Å	μ = 1.32 mm^{-1}
c = 15.0440 (14) Å	T = 291 (2) K
β = 104.6100 (10)º	Block, blue
V = 1879.2 (3) Å^3	0.36 × 0.27 × 0.24 mm
Z = 4	

Data collection

SMART CCD area-detector diffractometer	3499 independent reflections
Radiation source: fine-focus sealed tube	2627 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.021
T = 291(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −9→9
T_{min} = 0.634, T_{max} = 0.727	k = −19→19
14114 measured reflections	l = −18→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.040	H-atom parameters constrained
$wR(F^2)$ = 0.118	$w = 1/[\sigma^2(F_o^2) + (0.0601P)^2 + 0.8256P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
3499 reflections	$\Delta\rho_{max}$ = 0.55 e Å^{-3}
246 parameters	$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.25490 (5)	0.18713 (2)	0.62658 (3)	0.06726 (17)
Cl1	0.51574 (12)	0.20729 (7)	0.72554 (7)	0.0892 (3)
O1	0.0325 (3)	0.23262 (14)	0.6526 (2)	0.0883 (7)
O2	0.1888 (4)	0.30772 (16)	0.5907 (2)	0.1047 (9)
N1	0.2118 (3)	0.06795 (16)	0.6532 (2)	0.0692 (7)
N2	0.2893 (3)	0.13257 (18)	0.50468 (17)	0.0654 (7)
C1	0.3686 (5)	0.2577 (3)	0.4339 (3)	0.0989 (13)
H1A	0.2619	0.2872	0.4191	0.148*
H1B	0.4306	0.2704	0.3890	0.148*
H1C	0.4344	0.2747	0.4936	0.148*
C2	0.3361 (4)	0.1660 (3)	0.4340 (2)	0.0798 (10)
C3	0.3579 (5)	0.1140 (4)	0.3609 (3)	0.1068 (15)
H3	0.3925	0.1375	0.3120	0.128*
C4	0.3290 (5)	0.0311 (4)	0.3621 (3)	0.1126 (17)
H4	0.3411	−0.0019	0.3132	0.135*
C5	0.2808 (4)	−0.0064 (3)	0.4361 (3)	0.0914 (12)
C6	0.2490 (6)	−0.0936 (3)	0.4431 (4)	0.1109 (17)
H6	0.2599	−0.1295	0.3961	0.133*
C7	0.2039 (6)	−0.1248 (3)	0.5157 (4)	0.1129 (17)
H7	0.1829	−0.1821	0.5178	0.135*
C8	0.1869 (4)	−0.0736 (2)	0.5896 (3)	0.0878 (12)
C9	0.1446 (5)	−0.1015 (3)	0.6678 (4)	0.1085 (15)
H9	0.1211	−0.1580	0.6738	0.130*
C10	0.1370 (6)	−0.0480 (3)	0.7348 (4)	0.1115 (15)
H10	0.1088	−0.0679	0.7872	0.134*
C11	0.1711 (5)	0.0386 (2)	0.7277 (3)	0.0916 (11)
C12	0.1657 (7)	0.0984 (3)	0.8021 (3)	0.1284 (19)
H12A	0.2645	0.1340	0.8135	0.193*
H12B	0.1647	0.0680	0.8570	0.193*
H12C	0.0645	0.1321	0.7842	0.193*
C13	0.2195 (4)	0.0140 (2)	0.5848 (3)	0.0703 (9)
C14	0.2637 (4)	0.0475 (2)	0.5068 (2)	0.0702 (9)
C15	0.0574 (4)	0.30065 (18)	0.6177 (2)	0.0618 (7)
C16	−0.0696 (4)	0.36993 (19)	0.60953 (19)	0.0636 (7)
C17	−0.2333 (4)	0.3520 (3)	0.6138 (2)	0.0802 (10)
H17	−0.2644	0.2972	0.6234	0.096*
C18	−0.3518 (5)	0.4165 (3)	0.6036 (3)	0.1022 (13)
H18	−0.4641	0.4044	0.6037	0.123*
C19	−0.3057 (7)	0.4971 (3)	0.5935 (3)	0.1080 (14)
H19	−0.3858	0.5399	0.5882	0.130*
C20	−0.1434 (7)	0.5157 (3)	0.5911 (3)	0.1134 (15)
H20	−0.1113	0.5712	0.5859	0.136*
C21	−0.0254 (5)	0.4515 (2)	0.5965 (3)	0.0924 (11)

H21	0.0840	0.4637	0.5912	0.111*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0660 (3)	0.0575 (2)	0.0816 (3)	0.00553 (17)	0.0248 (2)	0.00678 (18)
Cl1	0.0797 (6)	0.0941 (7)	0.0833 (6)	−0.0101 (5)	0.0008 (4)	−0.0077 (5)
O1	0.0784 (15)	0.0559 (14)	0.136 (2)	0.0059 (11)	0.0374 (15)	0.0078 (14)
O2	0.104 (2)	0.0773 (17)	0.156 (3)	0.0294 (14)	0.0753 (19)	0.0437 (16)
N1	0.0591 (14)	0.0613 (15)	0.0919 (19)	0.0120 (12)	0.0276 (13)	0.0080 (14)
N2	0.0464 (13)	0.0868 (19)	0.0587 (15)	0.0011 (12)	0.0053 (11)	−0.0053 (13)
C1	0.088 (3)	0.136 (4)	0.073 (2)	−0.009 (3)	0.0217 (19)	0.023 (2)
C2	0.0550 (18)	0.120 (3)	0.0585 (19)	−0.0011 (18)	0.0035 (15)	−0.005 (2)
C3	0.070 (2)	0.185 (5)	0.061 (2)	0.000 (3)	0.0065 (17)	−0.010 (3)
C4	0.075 (3)	0.166 (5)	0.083 (3)	0.019 (3)	−0.005 (2)	−0.051 (3)
C5	0.056 (2)	0.114 (3)	0.088 (3)	0.0143 (19)	−0.0118 (18)	−0.034 (2)
C6	0.082 (3)	0.095 (3)	0.129 (4)	0.019 (2)	−0.022 (3)	−0.055 (3)
C7	0.078 (3)	0.077 (3)	0.154 (5)	0.007 (2)	−0.027 (3)	−0.029 (3)
C8	0.0470 (17)	0.070 (2)	0.130 (3)	0.0055 (15)	−0.008 (2)	−0.008 (2)
C9	0.068 (2)	0.082 (3)	0.166 (5)	−0.002 (2)	0.012 (3)	0.030 (3)
C10	0.096 (3)	0.096 (3)	0.154 (4)	0.013 (3)	0.054 (3)	0.046 (3)
C11	0.086 (2)	0.080 (2)	0.121 (3)	0.018 (2)	0.049 (2)	0.028 (2)
C12	0.176 (5)	0.116 (4)	0.123 (4)	0.040 (3)	0.095 (4)	0.039 (3)
C13	0.0426 (15)	0.065 (2)	0.095 (2)	0.0062 (13)	0.0038 (15)	−0.0020 (18)
C14	0.0411 (15)	0.081 (2)	0.077 (2)	0.0106 (14)	−0.0052 (14)	−0.0212 (18)
C15	0.0630 (18)	0.0551 (18)	0.0635 (18)	−0.0012 (13)	0.0090 (14)	−0.0038 (14)
C16	0.0710 (19)	0.0636 (18)	0.0524 (16)	0.0075 (15)	0.0087 (14)	−0.0029 (13)
C17	0.071 (2)	0.082 (2)	0.087 (2)	0.0052 (18)	0.0190 (18)	−0.0189 (19)
C18	0.080 (3)	0.117 (4)	0.112 (3)	0.020 (2)	0.027 (2)	−0.019 (3)
C19	0.112 (4)	0.102 (3)	0.110 (3)	0.046 (3)	0.030 (3)	−0.001 (3)
C20	0.123 (4)	0.077 (3)	0.145 (4)	0.033 (3)	0.042 (3)	0.029 (3)
C21	0.090 (3)	0.071 (2)	0.120 (3)	0.0204 (19)	0.035 (2)	0.022 (2)

Geometric parameters (Å, °)

Cu1—N1	1.990 (3)	C7—C8	1.414 (6)
Cu1—O2	2.031 (2)	C7—H7	0.9300
Cu1—O1	2.069 (2)	C8—C9	1.379 (6)
Cu1—N2	2.111 (3)	C8—C13	1.426 (5)
Cu1—Cl1	2.2795 (10)	C9—C10	1.334 (7)
Cu1—C15	2.396 (3)	C9—H9	0.9300
O1—C15	1.243 (4)	C10—C11	1.417 (6)
O2—C15	1.236 (4)	C10—H10	0.9300
N1—C11	1.330 (5)	C11—C12	1.480 (6)
N1—C13	1.356 (4)	C12—H12A	0.9600
N2—C2	1.328 (4)	C12—H12B	0.9600
N2—C14	1.374 (4)	C12—H12C	0.9600
C1—C2	1.485 (5)	C13—C14	1.414 (5)
C1—H1A	0.9600	C15—C16	1.493 (4)

C1—H1B	0.9600	C16—C17	1.374 (5)
C1—H1C	0.9600	C16—C21	1.376 (5)
C2—C3	1.424 (6)	C17—C18	1.389 (5)
C3—C4	1.342 (7)	C17—H17	0.9300
C3—H3	0.9300	C18—C19	1.357 (6)
C4—C5	1.402 (7)	C18—H18	0.9300
C4—H4	0.9300	C19—C20	1.357 (6)
C5—C14	1.401 (5)	C19—H19	0.9300
C5—C6	1.423 (6)	C20—C21	1.388 (5)
C6—C7	1.333 (7)	C20—H20	0.9300
C6—H6	0.9300	C21—H21	0.9300
N1—Cu1—O2	155.33 (11)	C9—C8—C13	116.6 (4)
N1—Cu1—O1	95.23 (10)	C7—C8—C13	117.9 (5)
O2—Cu1—O1	62.29 (10)	C10—C9—C8	120.5 (4)
N1—Cu1—N2	81.37 (12)	C10—C9—H9	119.8
O2—Cu1—N2	104.05 (12)	C8—C9—H9	119.8
O1—Cu1—N2	128.40 (10)	C9—C10—C11	121.3 (5)
N1—Cu1—Cl1	100.58 (8)	C9—C10—H10	119.4
O2—Cu1—Cl1	100.31 (11)	C11—C10—H10	119.4
O1—Cu1—Cl1	122.31 (8)	N1—C11—C10	120.0 (4)
N2—Cu1—Cl1	108.78 (7)	N1—C11—C12	118.2 (4)
N1—Cu1—C15	125.70 (10)	C10—C11—C12	121.8 (4)
O2—Cu1—C15	31.05 (10)	C11—C12—H12A	109.5
O1—Cu1—C15	31.25 (9)	C11—C12—H12B	109.5
N2—Cu1—C15	119.69 (10)	H12A—C12—H12B	109.5
Cl1—Cu1—C15	115.18 (8)	C11—C12—H12C	109.5
C15—O1—Cu1	89.06 (19)	H12A—C12—H12C	109.5
C15—O2—Cu1	91.0 (2)	H12B—C12—H12C	109.5
C11—N1—C13	119.1 (3)	N1—C13—C14	117.4 (3)
C11—N1—Cu1	126.7 (3)	N1—C13—C8	122.5 (4)
C13—N1—Cu1	114.1 (2)	C14—C13—C8	120.1 (4)
C2—N2—C14	119.4 (3)	N2—C14—C5	122.8 (4)
C2—N2—Cu1	131.1 (3)	N2—C14—C13	117.6 (3)
C14—N2—Cu1	109.4 (2)	C5—C14—C13	119.5 (4)
C2—C1—H1A	109.5	O2—C15—O1	117.6 (3)
C2—C1—H1B	109.5	O2—C15—C16	122.5 (3)
H1A—C1—H1B	109.5	O1—C15—C16	119.9 (3)
C2—C1—H1C	109.5	O2—C15—Cu1	57.96 (16)
H1A—C1—H1C	109.5	O1—C15—Cu1	59.69 (16)
H1B—C1—H1C	109.5	C16—C15—Cu1	178.1 (2)
N2—C2—C3	120.0 (4)	C17—C16—C21	119.5 (3)
N2—C2—C1	118.9 (3)	C17—C16—C15	119.7 (3)
C3—C2—C1	121.1 (4)	C21—C16—C15	120.8 (3)
C4—C3—C2	120.5 (4)	C16—C17—C18	119.2 (4)
C4—C3—H3	119.8	C16—C17—H17	120.4
C2—C3—H3	119.8	C18—C17—H17	120.4
C3—C4—C5	121.0 (4)	C19—C18—C17	120.8 (4)
C3—C4—H4	119.5	C19—C18—H18	119.6
C5—C4—H4	119.5	C17—C18—H18	119.6

C14—C5—C4	116.3 (4)	C20—C19—C18	120.3 (4)
C14—C5—C6	119.2 (5)	C20—C19—H19	119.8
C4—C5—C6	124.5 (5)	C18—C19—H19	119.8
C7—C6—C5	121.2 (5)	C19—C20—C21	119.6 (4)
C7—C6—H6	119.4	C19—C20—H20	120.2
C5—C6—H6	119.4	C21—C20—H20	120.2
C6—C7—C8	122.1 (5)	C16—C21—C20	120.3 (4)
C6—C7—H7	119.0	C16—C21—H21	119.8
C8—C7—H7	119.0	C20—C21—H21	119.8
C9—C8—C7	125.4 (5)		
N1—Cu1—O1—C15	−168.1 (2)	Cu1—N1—C11—C12	−3.8 (5)
O2—Cu1—O1—C15	1.2 (2)	C9—C10—C11—N1	−0.1 (7)
N2—Cu1—O1—C15	−85.0 (2)	C9—C10—C11—C12	−179.1 (5)
Cl1—Cu1—O1—C15	85.9 (2)	C11—N1—C13—C14	−179.8 (3)
N1—Cu1—O2—C15	25.0 (5)	Cu1—N1—C13—C14	2.8 (3)
O1—Cu1—O2—C15	−1.2 (2)	C11—N1—C13—C8	−0.5 (5)
N2—Cu1—O2—C15	125.1 (2)	Cu1—N1—C13—C8	−177.9 (2)
Cl1—Cu1—O2—C15	−122.4 (2)	C9—C8—C13—N1	0.7 (5)
O2—Cu1—N1—C11	−74.0 (4)	C7—C8—C13—N1	−178.0 (3)
O1—Cu1—N1—C11	−50.8 (3)	C9—C8—C13—C14	−180.0 (3)
N2—Cu1—N1—C11	−178.9 (3)	C7—C8—C13—C14	1.3 (4)
Cl1—Cu1—N1—C11	73.4 (3)	C2—N2—C14—C5	−1.6 (4)
C15—Cu1—N1—C11	−58.4 (3)	Cu1—N2—C14—C5	−178.7 (2)
O2—Cu1—N1—C13	103.2 (3)	C2—N2—C14—C13	177.9 (3)
O1—Cu1—N1—C13	126.3 (2)	Cu1—N2—C14—C13	0.8 (3)
N2—Cu1—N1—C13	−1.8 (2)	C4—C5—C14—N2	1.0 (4)
Cl1—Cu1—N1—C13	−109.4 (2)	C6—C5—C14—N2	−178.9 (3)
C15—Cu1—N1—C13	118.8 (2)	C4—C5—C14—C13	−178.5 (3)
N1—Cu1—N2—C2	−176.2 (3)	C6—C5—C14—C13	1.6 (5)
O2—Cu1—N2—C2	28.4 (3)	N1—C13—C14—N2	−2.4 (4)
O1—Cu1—N2—C2	94.0 (3)	C8—C13—C14—N2	178.3 (3)
Cl1—Cu1—N2—C2	−77.9 (3)	N1—C13—C14—C5	177.2 (3)
C15—Cu1—N2—C2	57.5 (3)	C8—C13—C14—C5	−2.2 (4)
N1—Cu1—N2—C14	0.52 (18)	Cu1—O2—C15—O1	2.0 (3)
O2—Cu1—N2—C14	−154.91 (19)	Cu1—O2—C15—C16	−177.8 (3)
O1—Cu1—N2—C14	−89.3 (2)	Cu1—O1—C15—O2	−2.0 (3)
Cl1—Cu1—N2—C14	98.83 (17)	Cu1—O1—C15—C16	177.8 (2)
C15—Cu1—N2—C14	−125.84 (18)	N1—Cu1—C15—O2	−167.4 (2)
C14—N2—C2—C3	0.5 (4)	O1—Cu1—C15—O2	177.9 (4)
Cu1—N2—C2—C3	177.0 (2)	N2—Cu1—C15—O2	−66.1 (3)
C14—N2—C2—C1	−178.1 (3)	Cl1—Cu1—C15—O2	66.6 (3)
Cu1—N2—C2—C1	−1.7 (4)	N1—Cu1—C15—O1	14.6 (2)
N2—C2—C3—C4	1.0 (6)	O2—Cu1—C15—O1	−177.9 (4)
C1—C2—C3—C4	179.6 (4)	N2—Cu1—C15—O1	116.0 (2)
C2—C3—C4—C5	−1.6 (6)	Cl1—Cu1—C15—O1	−111.34 (19)
C3—C4—C5—C14	0.6 (6)	O2—C15—C16—C17	160.2 (3)
C3—C4—C5—C6	−179.5 (4)	O1—C15—C16—C17	−19.6 (4)
C14—C5—C6—C7	−0.2 (6)	O2—C15—C16—C21	−18.9 (5)
C4—C5—C6—C7	179.9 (4)	O1—C15—C16—C21	161.3 (3)

C5—C6—C7—C8	−0.7 (7)	C21—C16—C17—C18	0.9 (5)
C6—C7—C8—C9	−178.5 (4)	C15—C16—C17—C18	−178.3 (3)
C6—C7—C8—C13	0.1 (6)	C16—C17—C18—C19	−2.8 (6)
C7—C8—C9—C10	178.0 (4)	C17—C18—C19—C20	1.5 (7)
C13—C8—C9—C10	−0.6 (6)	C18—C19—C20—C21	1.8 (8)
C8—C9—C10—C11	0.3 (7)	C17—C16—C21—C20	2.4 (6)
C13—N1—C11—C10	0.2 (5)	C15—C16—C21—C20	−178.5 (4)
Cu1—N1—C11—C10	177.2 (3)	C19—C20—C21—C16	−3.8 (7)
C13—N1—C11—C12	179.2 (3)		

Fig. 1

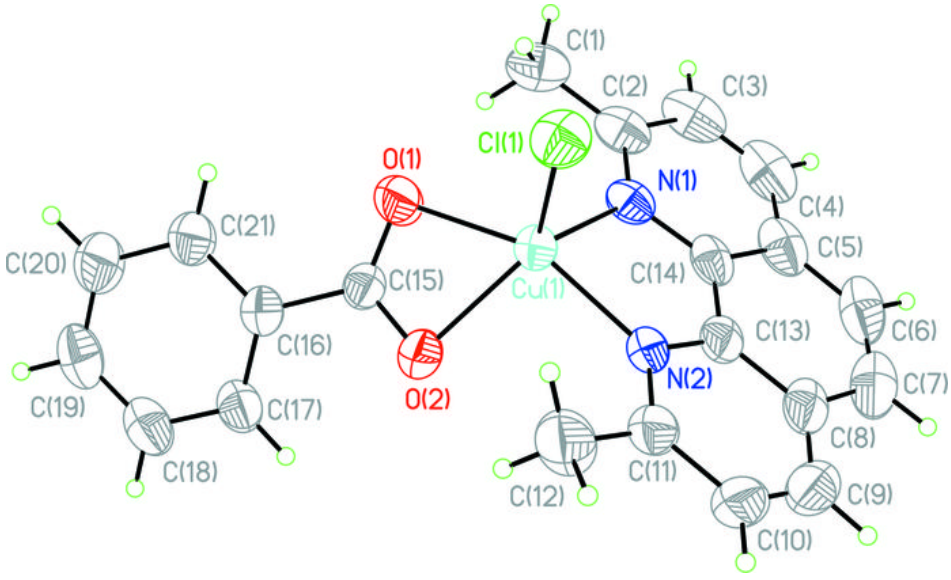

C(1)
C(2)
C(3)
Cl(1)
O(1)
N(1)
C(4)
C(5)
C(21)
C(20)
C(15)
Cu(1)
C(14)
C(16)
C(13)
C(6)
O(2)
N(2)
C(7)
C(19)
C(17)
C(8)
C(18)
C(11)
C(12)
C(9)
C(10)

Fig. 2