

catena-Poly[[[2-[3-(dimethylamino)-propyliminomethyl]-4-nitrophenolato]-copper(II)]- μ -acetato]

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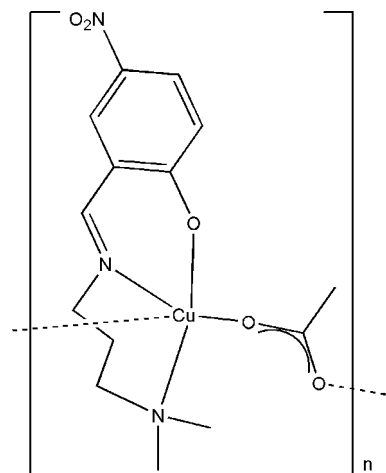
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.079; wR factor = 0.184; data-to-parameter ratio = 16.7.

The title compound, $[\text{Cu}(\text{C}_{12}\text{H}_{16}\text{N}_3\text{O}_3)(\text{CH}_3\text{COO})]_n$ or $[\text{Cu}(\text{CMP})(\text{CH}_3\text{COO})]_n$ {CMP is 2-[3-(dimethylamino)propyliminomethyl]-4-nitrophenol}, was synthesized by the reaction of 2-hydroxy-5-nitrobenzaldehyde, *N,N*-dimethylpropane-1,3-diamine and copper(II) acetate monohydrate in a methanol solution. The compound is an acetate-bridged polymeric copper(II) complex. The Cu^{II} atom is coordinated in a square-pyramidal manner by one Schiff base CMP ligand and two acetate anions. The Schiff base molecule acts as a tridentate ligand, coordinating the Cu^{II} ion through its phenolate O atom, imine N atom and amine N atom. The acetate anion acts as a bridging group, coordinating two adjacent Cu^{II} ions through its two O atoms, one in the basal plane and the other in the apical position. The $[\text{Cu}(\text{CMP})]$ units are linked through the bridging acetate groups, forming chains running along the c axis.

Related literature

For azido-bridged polynuclear complexes, see: Escuer & Aromí (2006); Massoud *et al.* (2007). For thiocyanato-bridged polynuclear complexes, see: Zhang *et al.* (2001); Dey *et al.* (2004). For cyano-bridged polynuclear complexes, see: Liu *et al.* (2006); Mondal *et al.* (2001). For our previously reported Schiff base complexes, see: Li (2007*a,b*). For related structures, see: Hebbachi & Benali-Cherif (2005); Wang & You (2007); Diao *et al.* (2007); Usman *et al.* (2003).



Experimental

Crystal data

$[\text{Cu}(\text{C}_{12}\text{H}_{16}\text{N}_3\text{O}_3)(\text{C}_2\text{H}_3\text{O}_2)]$
 $M_r = 372.86$
 Monoclinic, $P2_1/c$
 $a = 13.834$ (3) Å
 $b = 11.661$ (2) Å
 $c = 9.988$ (2) Å
 $\beta = 99.86$ (3)°

$V = 1587.5$ (6) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.41$ mm⁻¹
 $T = 298$ (2) K
 0.27 × 0.23 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.703$, $T_{\text{max}} = 0.767$

9081 measured reflections
 3522 independent reflections
 2037 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.087$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.079$
 $wR(F^2) = 0.184$
 $S = 1.00$
 3522 reflections

211 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.85$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.61$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1—O3	1.946 (4)	Cu1—N2	2.091 (5)
Cu1—O4	1.965 (4)	Cu1—O5 ⁱ	2.265 (4)
Cu1—N1	1.992 (5)		
O3—Cu1—O4	87.07 (17)	N1—Cu1—N2	93.3 (2)
O3—Cu1—N1	90.17 (18)	O3—Cu1—O5 ⁱ	92.62 (16)
O4—Cu1—N1	161.58 (19)	O4—Cu1—O5 ⁱ	107.21 (17)
O3—Cu1—N2	173.93 (19)	N1—Cu1—O5 ⁱ	91.10 (18)
O4—Cu1—N2	88.09 (19)	N2—Cu1—O5 ⁱ	92.32 (18)

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

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997*a*); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997*a*); molecular graphics: SHELXTL (Sheldrick, 1997*b*); software used to prepare material for publication: SHELXTL.

The author gratefully acknowledges Jingchu University of Technology for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2461).

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supplementary materials

Acta Cryst. (2007). E63, m2982-m2983 [doi:10.1107/S1600536807057376]

***catena*-Poly[[{2-[3-(dimethylamino)propyliminomethyl]-4-nitrophenolato}copper(II)]- μ -acetato]**

W.-H. Li

Comment

Polynuclear complexes are very interesting in both structures and properties in coordination chemistry. The azide, thiocyanate, and cyanide anions are often used to construct versatile polynuclear complexes (Escuer & Aromí, 2006; Mas-soud *et al.*, 2007; Zhang *et al.*, 2001; Dey *et al.*, 2004; Liu *et al.*, 2006; Mondal *et al.*, 2001). In comparison, the acetato-bridged polynuclear complexes are rarely seen. Recently, we have reported the crystal structures of some Schiff base complexes (Li, 2007*a,b*). In order to investigate the coordination modes of the acetate anions, the author reports herein the crystal structure of an acetato-bridged polynuclear copper(II) complex with Schiff base ligand 4-chloro-2-[(3-dimethylaminopropylimino)methyl]phenol (CMP).

The Cu atom in the acetato-bridged polynuclear complex is square-pyramidal coordinated by one Schiff base ligand CMP and two acetate anions (Fig. 1). The Schiff base molecule acts as a tridentate ligand coordinating the copper ion through the phenolic O atom, imine N atom and amine N atom. The acetate anion acts as a bridging group coordinating adjacent two copper ions through the two O atoms, one at the basal plane and the other one at the apical position. All the coordinated bond lengths and angles (Table 1) are comparable to the values in other similar Schiff base copper(II) complexes (Hebbachi & Benali-Cherif, 2005; Wang & You, 2007; Diao *et al.*, 2007; Usman *et al.*, 2003).

In the crystal structure, the [Cu(CMP)] units are linked through the bridging acetate groups, forming chains running along the *c* axis (Fig. 2).

Experimental

5-Nitro-2-hydroxybenzaldehyde (0.1 mmol, 16.7 mg), *N,N*-dimethylpropane-1,3-diamine (0.1 mmol, 10.2 mg), and copper(II) acetate monohydrate (0.1 mmol, 19.9 mg) were mixed in methanol (20 ml) and the mixture was stirred for 30 min at room temperature. The reaction mixture was filtered. Blue block-shaped single crystals suitable for X-ray diffraction were formed from the filtrate after a week.

Refinement

All H atom positions were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, with $U_{\text{iso}}(\text{H})$ values set at $1.2U_{\text{eq}}(\text{C})$ and $1.5U_{\text{eq}}(\text{methyl C})$.

Figures

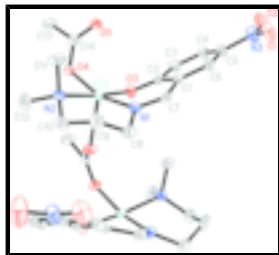


Fig. 1. The molecular structure of (I), shown with 30% probability displacement ellipsoids.

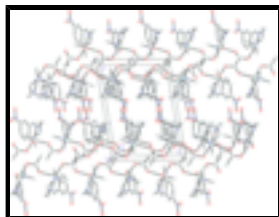


Fig. 2. Molecular packing of (I).

catena-Poly[[{2-[3-(dimethylamino)propyliminomethyl]-4- nitrophenolato}copper(II)]- μ -acetato]

Crystal data

[Cu(C₁₂H₁₆N₃O₃)(C₂H₃O₂)]

$M_r = 372.86$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 13.834 (3) \text{ \AA}$

$b = 11.661 (2) \text{ \AA}$

$c = 9.988 (2) \text{ \AA}$

$\beta = 99.86 (3)^\circ$

$V = 1587.5 (6) \text{ \AA}^3$

$Z = 4$

$F_{000} = 772$

$D_x = 1.560 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1027 reflections

$\theta = 2.3\text{--}24.5^\circ$

$\mu = 1.41 \text{ mm}^{-1}$

$T = 298 (2) \text{ K}$

Block, blue

$0.27 \times 0.23 \times 0.20 \text{ mm}$

Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298(2) \text{ K}$

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.703$, $T_{\max} = 0.767$

9081 measured reflections

3522 independent reflections

2037 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.087$

$\theta_{\max} = 27.5^\circ$

$\theta_{\min} = 1.5^\circ$

$h = -17 \rightarrow 17$

$k = -15 \rightarrow 12$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.079$	H-atom parameters constrained
$wR(F^2) = 0.184$	$w = 1/[\sigma^2(F_o^2) + (0.0706P)^2]$
$S = 1.00$	where $P = (F_o^2 + 2F_c^2)/3$
3522 reflections	$(\Delta/\sigma)_{\max} < 0.001$
211 parameters	$\Delta\rho_{\max} = 0.85 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.61 \text{ e } \text{\AA}^{-3}$
	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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.82621 (5)	0.77042 (6)	0.15549 (7)	0.0297 (3)
O1	0.4913 (4)	0.3131 (5)	0.2555 (6)	0.0722 (16)
O2	0.6056 (5)	0.1905 (6)	0.3039 (8)	0.105 (3)
O3	0.8450 (3)	0.6052 (4)	0.1489 (4)	0.0371 (11)
O4	0.9473 (3)	0.7753 (4)	0.2908 (4)	0.0368 (10)
O5	0.8694 (3)	0.7033 (4)	0.4489 (4)	0.0398 (11)
N1	0.6858 (4)	0.7516 (4)	0.0710 (5)	0.0359 (13)
N2	0.8117 (4)	0.9467 (4)	0.1846 (5)	0.0375 (13)
N3	0.5767 (5)	0.2850 (6)	0.2657 (7)	0.0584 (17)
C1	0.6773 (4)	0.5540 (5)	0.1479 (6)	0.0331 (14)
C2	0.7805 (4)	0.5326 (5)	0.1707 (5)	0.0301 (14)
C3	0.8105 (5)	0.4200 (6)	0.2173 (6)	0.0438 (17)
H3	0.8766	0.4006	0.2282	0.053*
C4	0.7456 (5)	0.3407 (6)	0.2461 (7)	0.0453 (17)
H4	0.7677	0.2688	0.2781	0.054*
C5	0.6451 (5)	0.3667 (6)	0.2278 (6)	0.0401 (16)
C6	0.6122 (5)	0.4719 (5)	0.1788 (6)	0.0384 (15)
H6	0.5455	0.4884	0.1661	0.046*

supplementary materials

C7	0.6381 (4)	0.6600 (6)	0.0865 (6)	0.0363 (15)
H7	0.5708	0.6619	0.0547	0.044*
C8	0.6331 (5)	0.8417 (6)	-0.0144 (7)	0.0504 (19)
H8A	0.5644	0.8207	-0.0362	0.061*
H8B	0.6585	0.8453	-0.0991	0.061*
C9	0.6408 (5)	0.9577 (6)	0.0489 (7)	0.055 (2)
H9A	0.6170	0.9539	0.1347	0.065*
H9B	0.5986	1.0102	-0.0099	0.065*
C10	0.7438 (5)	1.0050 (6)	0.0742 (7)	0.0496 (18)
H10A	0.7706	0.9991	-0.0092	0.060*
H10B	0.7410	1.0858	0.0964	0.060*
C11	0.7785 (6)	0.9636 (6)	0.3160 (6)	0.057 (2)
H11A	0.7702	1.0440	0.3311	0.085*
H11B	0.8266	0.9329	0.3878	0.085*
H11C	0.7172	0.9248	0.3147	0.085*
C12	0.9085 (5)	1.0048 (6)	0.1915 (8)	0.056 (2)
H12A	0.9020	1.0846	0.2119	0.084*
H12B	0.9303	0.9972	0.1057	0.084*
H12C	0.9556	0.9700	0.2615	0.084*
C13	1.0367 (5)	0.7595 (6)	0.5095 (7)	0.054 (2)
H13A	1.0349	0.8321	0.5545	0.081*
H13B	1.0914	0.7581	0.4619	0.081*
H13C	1.0437	0.6990	0.5757	0.081*
C14	0.9432 (5)	0.7429 (5)	0.4103 (6)	0.0332 (15)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0299 (4)	0.0322 (5)	0.0270 (4)	-0.0009 (3)	0.0052 (3)	0.0021 (3)
O1	0.057 (4)	0.059 (4)	0.109 (5)	-0.012 (3)	0.038 (3)	0.006 (3)
O2	0.086 (5)	0.052 (4)	0.183 (7)	-0.002 (4)	0.043 (5)	0.040 (5)
O3	0.032 (2)	0.032 (3)	0.048 (3)	-0.0026 (19)	0.0119 (19)	-0.008 (2)
O4	0.044 (2)	0.041 (3)	0.025 (2)	-0.003 (2)	0.0045 (17)	0.004 (2)
O5	0.038 (2)	0.054 (3)	0.029 (2)	-0.006 (2)	0.0133 (18)	0.001 (2)
N1	0.034 (3)	0.040 (4)	0.033 (3)	-0.001 (2)	0.006 (2)	0.006 (2)
N2	0.050 (3)	0.032 (3)	0.033 (3)	0.002 (2)	0.013 (2)	0.002 (2)
N3	0.059 (4)	0.040 (4)	0.081 (5)	-0.002 (3)	0.024 (4)	0.000 (4)
C1	0.047 (4)	0.028 (4)	0.026 (3)	-0.005 (3)	0.009 (3)	-0.007 (3)
C2	0.033 (3)	0.030 (4)	0.028 (3)	-0.001 (3)	0.006 (2)	-0.010 (3)
C3	0.049 (4)	0.036 (4)	0.046 (4)	0.005 (3)	0.004 (3)	0.001 (3)
C4	0.054 (4)	0.029 (4)	0.052 (4)	0.000 (3)	0.007 (3)	0.001 (3)
C5	0.049 (4)	0.031 (4)	0.043 (4)	-0.006 (3)	0.015 (3)	-0.005 (3)
C6	0.038 (3)	0.036 (4)	0.043 (4)	-0.007 (3)	0.012 (3)	-0.010 (3)
C7	0.030 (3)	0.046 (4)	0.032 (3)	-0.007 (3)	0.001 (3)	-0.003 (3)
C8	0.052 (4)	0.051 (5)	0.044 (4)	0.003 (3)	-0.004 (3)	0.008 (4)
C9	0.052 (4)	0.044 (5)	0.061 (5)	0.003 (4)	-0.009 (4)	0.022 (4)
C10	0.063 (5)	0.035 (4)	0.052 (4)	0.007 (3)	0.012 (4)	0.011 (3)
C11	0.082 (6)	0.055 (5)	0.033 (4)	0.021 (4)	0.009 (4)	0.006 (4)

C12	0.054 (4)	0.035 (4)	0.074 (5)	-0.007 (3)	0.000 (4)	0.003 (4)
C13	0.051 (4)	0.081 (6)	0.031 (3)	-0.003 (4)	0.007 (3)	-0.001 (4)
C14	0.036 (3)	0.032 (4)	0.031 (3)	0.008 (3)	0.005 (3)	-0.001 (3)

Geometric parameters (Å, °)

Cu1—O3	1.946 (4)	C4—C5	1.404 (9)
Cu1—O4	1.965 (4)	C4—H4	0.9300
Cu1—N1	1.992 (5)	C5—C6	1.370 (9)
Cu1—N2	2.091 (5)	C6—H6	0.9300
Cu1—O5 ⁱ	2.265 (4)	C7—H7	0.9300
O1—N3	1.215 (8)	C8—C9	1.490 (10)
O2—N3	1.211 (8)	C8—H8A	0.9700
O3—C2	1.276 (7)	C8—H8B	0.9700
O4—C14	1.262 (7)	C9—C10	1.509 (9)
O5—C14	1.241 (7)	C9—H9A	0.9700
O5—Cu1 ⁱⁱ	2.265 (4)	C9—H9B	0.9700
N1—C7	1.280 (7)	C10—H10A	0.9700
N1—C8	1.467 (8)	C10—H10B	0.9700
N2—C11	1.476 (8)	C11—H11A	0.9600
N2—C10	1.485 (8)	C11—H11B	0.9600
N2—C12	1.492 (8)	C11—H11C	0.9600
N3—C5	1.438 (9)	C12—H12A	0.9600
C1—C6	1.385 (8)	C12—H12B	0.9600
C1—C2	1.429 (8)	C12—H12C	0.9600
C1—C7	1.444 (9)	C13—C14	1.502 (9)
C2—C3	1.431 (9)	C13—H13A	0.9600
C3—C4	1.353 (9)	C13—H13B	0.9600
C3—H3	0.9300	C13—H13C	0.9600
O3—Cu1—O4	87.07 (17)	N1—C7—C1	127.0 (6)
O3—Cu1—N1	90.17 (18)	N1—C7—H7	116.5
O4—Cu1—N1	161.58 (19)	C1—C7—H7	116.5
O3—Cu1—N2	173.93 (19)	N1—C8—C9	114.3 (5)
O4—Cu1—N2	88.09 (19)	N1—C8—H8A	108.7
N1—Cu1—N2	93.3 (2)	C9—C8—H8A	108.7
O3—Cu1—O5 ⁱ	92.62 (16)	N1—C8—H8B	108.7
O4—Cu1—O5 ⁱ	107.21 (17)	C9—C8—H8B	108.7
N1—Cu1—O5 ⁱ	91.10 (18)	H8A—C8—H8B	107.6
N2—Cu1—O5 ⁱ	92.32 (18)	C8—C9—C10	113.5 (6)
C2—O3—Cu1	123.4 (4)	C8—C9—H9A	108.9
C14—O4—Cu1	118.0 (4)	C10—C9—H9A	108.9
C14—O5—Cu1 ⁱⁱ	126.3 (4)	C8—C9—H9B	108.9
C7—N1—C8	116.9 (5)	C10—C9—H9B	108.9
C7—N1—Cu1	121.8 (4)	H9A—C9—H9B	107.7
C8—N1—Cu1	121.3 (4)	N2—C10—C9	114.6 (5)
C11—N2—C10	110.3 (5)	N2—C10—H10A	108.6
C11—N2—C12	108.2 (5)	C9—C10—H10A	108.6

supplementary materials

C10—N2—C12	105.9 (5)	N2—C10—H10B	108.6
C11—N2—Cu1	107.9 (4)	C9—C10—H10B	108.6
C10—N2—Cu1	114.2 (4)	H10A—C10—H10B	107.6
C12—N2—Cu1	110.2 (4)	N2—C11—H11A	109.5
O2—N3—O1	122.4 (7)	N2—C11—H11B	109.5
O2—N3—C5	119.3 (7)	H11A—C11—H11B	109.5
O1—N3—C5	118.3 (6)	N2—C11—H11C	109.5
C6—C1—C2	120.9 (6)	H11A—C11—H11C	109.5
C6—C1—C7	118.3 (6)	H11B—C11—H11C	109.5
C2—C1—C7	120.7 (6)	N2—C12—H12A	109.5
O3—C2—C1	124.4 (6)	N2—C12—H12B	109.5
O3—C2—C3	119.5 (6)	H12A—C12—H12B	109.5
C1—C2—C3	116.0 (6)	N2—C12—H12C	109.5
C4—C3—C2	122.0 (6)	H12A—C12—H12C	109.5
C4—C3—H3	119.0	H12B—C12—H12C	109.5
C2—C3—H3	119.0	C14—C13—H13A	109.5
C3—C4—C5	120.2 (6)	C14—C13—H13B	109.5
C3—C4—H4	119.9	H13A—C13—H13B	109.5
C5—C4—H4	119.9	C14—C13—H13C	109.5
C6—C5—C4	120.1 (6)	H13A—C13—H13C	109.5
C6—C5—N3	119.6 (6)	H13B—C13—H13C	109.5
C4—C5—N3	120.3 (6)	O5—C14—O4	125.4 (6)
C5—C6—C1	120.7 (6)	O5—C14—C13	120.3 (5)
C5—C6—H6	119.7	O4—C14—C13	114.3 (6)
C1—C6—H6	119.7		

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

Fig. 1

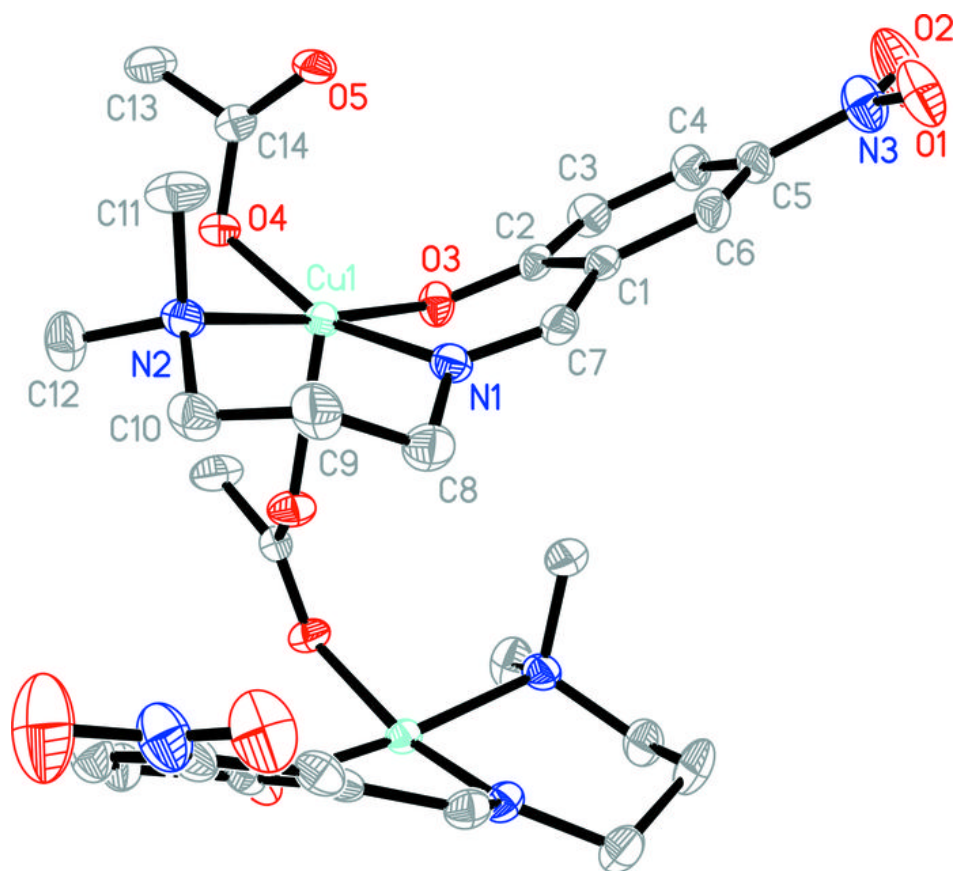


Fig. 2

