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# Bis{2-methoxy-6-[(3-methoxypropyl)-iminomethyl]phenolato-$\kappa^2N,O^1$}-copper(II)

**Amitabha Datta, Jui-Hsien Huang and Hon Man Lee***

National Changhua University of Education, Department of Chemistry, Changhua 50058, Taiwan
Correspondence e-mail: leehm@cc.ncue.edu.tw

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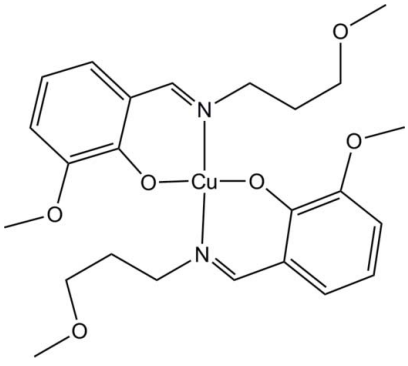
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.027; $wR$ factor = 0.079; data-to-parameter ratio = 15.0.

The title complex, $[Cu(C_{12}H_{16}NO_3)_2]$, adopts a distorted square-planar coordination geometry with the $Cu^{II}$ ion situated on a crystallographic inversion center. The two Schiff base ligands are coordinated in a *trans* fashion. In the crystal structure, non-classical intermolecular C—H···O hydrogen bonds involving the ether O atoms link the Schiff base molecules into a two-dimensional network parallel to (101).

## Related literature

For similar copper(II) structures with Schiff base ligands: see: Akitsu & Einaga (2004); Bluhm *et al.* (2003); Castiñeiras *et al.* (1990); Costamagna *et al.* (1998); King *et al.* (1973); Lacroix *et al.* (2004); Zhang *et al.* (2001).




## Experimental

### Crystal data

$[Cu(C_{12}H_{16}NO_3)_2]$ $M_r$ = 508.06
Monoclinic, $P2_1/c$
$a$ = 11.2189 (9) Å
$b$ = 10.7004 (8) Å
$c$ = 9.5002 (7) Å
$\beta$ = 96.912 (1)°
$V$ = 1132.18 (15) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.01 mm$^{-1}$
$T$ = 100 (2) K
0.50 × 0.50 × 0.40 mm

### Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.614, $T_{max}$ = 0.668
6343 measured reflections
2298 independent reflections
2065 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.079
$S$ = 1.09
2298 reflections
153 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8$B$···O3$^{i}$ | 0.98 | 2.58 | 3.476 (2) | 151 |
| C9—H9$A$···O1$^{ii}$ | 0.99 | 2.31 | 2.782 (2) | 108 |
| C9—H9$B$···O3 | 0.99 | 2.55 | 2.918 (2) | 102 |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: LH2719).

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# supplementary materials

*Acta Cryst.* (2008). E**64**, m1497 [ **doi:10.1107/S1600536808035289** ]

# Bis{2-methoxy-6-[(3-methoxypropyl)iminomethyl]phenolato-$\kappa^2N,O^1$}copper(II)

**A. Datta, J.-H. Huang and H. M. Lee**

## Comment

The Schiff base (*E*)-2-methoxy-6-[(3-methoxypropyl)iminomethyl]phenol reacts with copper(II) nitrate in methanol to form the title complex. In situ deprotonation of the phenolic hydrogen occurred leading to formation of the O/N-bidentate ligand. The title complex consists of two bidentate ligands coordinating in a *trans* fashion. It adopts a square-planar coordination geometry with the Cu atom located on a crystallographic inversion center. Schiff base Cu(II) complexes similar to the title complex have been reported in the literature (Akitsu & Einaga, 2004; Bluhm *et al.*, 2003; Castiñeiras *et al.*, 1990; Costamagna *et al.*, 1998; King *et al.*, 1973; Lacroix *et al.*, 2004; Zhang *et al.*, 2001).

Both intramolecular and intermolecular non-classical H-bonds of the type C-H···O exist (Table 1). The intermolecular H-bonds link the complex into a two-dimensional network.

## Experimental

Synthesis of (*E*)-2-methoxy-6-((3-methoxypropylimino)methyl)phenol: The compound was synthesized by the condensation reaction between O-vaniline and $NH_2(CH_2)_3OMe$ in methanol. After complete removal of the solvent, the resulting yellow liquid was used without purification.

Synthesis of the title complex: A methanolic solution of $Cu(NO_3)_2$ (1 mmol, 188 mg) and (*E*)-2-methoxy-6-((3-methoxypropylimino)methyl)phenol (2 mmol, 446 mg) was stirred for 30 min. The solution was then kept for 7 days to yield crystals suitable for X-ray diffraction study.

## Refinement

All the H atoms were positioned geometrically and refined as riding atoms, with $C_{aryl}$—H = 0.95, $C_{methyl}$—H = 0.98, $C_{methylene}$—H = 0.99, $C_{methine}$—H = 0.95 Å while $U_{iso}(H) = 1.5U_{eq}(C)$ for the methyl H atoms and $U_{iso}(H) = 1.2U_{eq}(C)$ for all the other H atoms.

## Figures

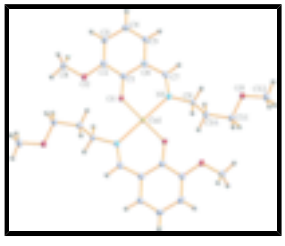

Fig. 1. The structure of the title complex, showing 50% displacement ellipsoids for non-H atoms. The H atoms are dipicted by circles of an arbitrary radius. The unlabelled atoms are related to the labelled ones by -*x*, 1 - *y*, 1 - *z*.

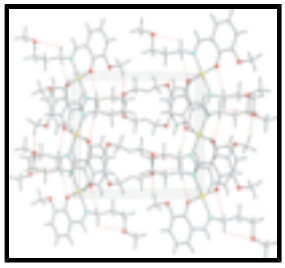

Fig. 2. A packing diagram of the title compound along the *c* axis. Hyrogen bonds are shown as dashed lines.

## Bis{2-methoxy-6-[(3-methoxypropyl)iminomethyl]phenolato- $\kappa^2N,O^1$}copper(II)

*Crystal data*

| | |
|---|---|
| $[Cu(C_{12}H_{16}N_1O_3)_2]$ | $F_{000}$ = 534 |
| $M_r$ = 508.06 | $D_x$ = 1.490 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 3703 reflections |
| $a$ = 11.2189 (9) Å | θ = 2.6–26.4º |
| $b$ = 10.7004 (8) Å | μ = 1.01 mm$^{-1}$ |
| $c$ = 9.5002 (7) Å | $T$ = 100 (2) K |
| β = 96.9120 (10)º | Block, black |
| $V$ = 1132.18 (15) Å$^3$ | 0.50 × 0.50 × 0.40 mm |
| $Z$ = 2 | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII diffractometer | 2065 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.032 |
| $T$ = 100(2) K | $\theta_{max}$ = 26.4º |
| ω scans | $\theta_{min}$ = 2.6º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −13→7 |
| $T_{min}$ = 0.614, $T_{max}$ = 0.668 | $k$ = −13→12 |
| 6343 measured reflections | $l$ = −11→11 |
| 2298 independent reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.027 | H-atom parameters constrained |
| $wR(F^2)$ = 0.079 | $w = 1/[\sigma^2(F_o^2) + (0.0461P)^2 + 0.0531P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.09 | $(\Delta/\sigma)_{max} < 0.001$ |

| | |
|---|---|
| 2298 reflections | $\Delta\rho_{max} = 0.31$ e Å$^{-3}$ |
| 153 parameters | $\Delta\rho_{min} = -0.37$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cu1 | 0.0000 | 0.5000 | 0.5000 | 0.01161 (11) |
| N1 | 0.06486 (12) | 0.67268 (12) | 0.54175 (13) | 0.0124 (3) |
| O1 | −0.10464 (10) | 0.55690 (11) | 0.34077 (12) | 0.0157 (3) |
| O2 | −0.26520 (10) | 0.57869 (11) | 0.11946 (12) | 0.0168 (3) |
| O3 | 0.38383 (10) | 0.83717 (11) | 0.73181 (13) | 0.0203 (3) |
| C1 | −0.12843 (14) | 0.67057 (15) | 0.29658 (16) | 0.0123 (3) |
| C2 | −0.21677 (14) | 0.68788 (15) | 0.17655 (16) | 0.0133 (3) |
| C3 | −0.24800 (15) | 0.80571 (16) | 0.12650 (17) | 0.0146 (3) |
| H3 | −0.3084 | 0.8153 | 0.0481 | 0.018* |
| C4 | −0.19103 (15) | 0.91184 (16) | 0.19081 (17) | 0.0160 (4) |
| H4 | −0.2131 | 0.9930 | 0.1564 | 0.019* |
| C5 | −0.10354 (15) | 0.89779 (15) | 0.30333 (17) | 0.0146 (3) |
| H5 | −0.0639 | 0.9695 | 0.3453 | 0.018* |
| C6 | −0.07147 (15) | 0.77820 (15) | 0.35771 (16) | 0.0128 (3) |
| C7 | 0.02158 (15) | 0.77112 (16) | 0.47516 (16) | 0.0134 (3) |
| H7 | 0.0557 | 0.8486 | 0.5081 | 0.016* |
| C8 | −0.35395 (15) | 0.59005 (17) | −0.00057 (17) | 0.0185 (4) |
| H8A | −0.4248 | 0.6325 | 0.0275 | 0.028* |
| H8B | −0.3767 | 0.5067 | −0.0372 | 0.028* |
| H8C | −0.3214 | 0.6388 | −0.0744 | 0.028* |
| C9 | 0.16306 (14) | 0.69566 (15) | 0.65644 (16) | 0.0136 (3) |
| H9A | 0.1512 | 0.6429 | 0.7392 | 0.016* |
| H9B | 0.1613 | 0.7842 | 0.6862 | 0.016* |
| C10 | 0.28466 (15) | 0.66641 (16) | 0.60836 (17) | 0.0166 (4) |
| H10A | 0.2902 | 0.5756 | 0.5904 | 0.020* |
| H10B | 0.2919 | 0.7107 | 0.5183 | 0.020* |
| C11 | 0.38687 (15) | 0.70517 (15) | 0.71811 (18) | 0.0161 (4) |
| H11A | 0.3781 | 0.6652 | 0.8103 | 0.019* |

| | | | | |
|---|---|---|---|---|
| H11B | 0.4645 | 0.6787 | 0.6881 | 0.019* |
| C12 | 0.47976 (15) | 0.88352 (17) | 0.82805 (18) | 0.0214 (4) |
| H12A | 0.4776 | 0.8444 | 0.9210 | 0.032* |
| H12B | 0.4719 | 0.9743 | 0.8369 | 0.032* |
| H12C | 0.5562 | 0.8639 | 0.7929 | 0.032* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cu1 | 0.01075 (17) | 0.01035 (17) | 0.01270 (16) | −0.00026 (10) | −0.00282 (11) | 0.00036 (10) |
| N1 | 0.0102 (7) | 0.0140 (7) | 0.0128 (6) | −0.0004 (6) | 0.0000 (6) | −0.0016 (6) |
| O1 | 0.0166 (6) | 0.0117 (6) | 0.0170 (6) | 0.0001 (5) | −0.0057 (5) | 0.0011 (5) |
| O2 | 0.0164 (6) | 0.0158 (6) | 0.0163 (6) | −0.0019 (5) | −0.0061 (5) | −0.0006 (5) |
| O3 | 0.0167 (6) | 0.0128 (6) | 0.0286 (7) | −0.0022 (5) | −0.0085 (5) | 0.0003 (5) |
| C1 | 0.0108 (8) | 0.0133 (8) | 0.0133 (7) | 0.0012 (7) | 0.0033 (6) | 0.0004 (6) |
| C2 | 0.0116 (8) | 0.0149 (8) | 0.0138 (7) | −0.0009 (7) | 0.0027 (7) | −0.0009 (6) |
| C3 | 0.0114 (8) | 0.0191 (9) | 0.0130 (7) | 0.0020 (7) | 0.0002 (6) | 0.0032 (7) |
| C4 | 0.0171 (9) | 0.0135 (8) | 0.0176 (8) | 0.0024 (7) | 0.0029 (7) | 0.0030 (7) |
| C5 | 0.0165 (9) | 0.0108 (8) | 0.0169 (8) | −0.0004 (7) | 0.0032 (7) | −0.0011 (7) |
| C6 | 0.0115 (8) | 0.0141 (8) | 0.0132 (8) | 0.0013 (7) | 0.0029 (7) | 0.0003 (6) |
| C7 | 0.0136 (8) | 0.0120 (8) | 0.0149 (8) | −0.0014 (6) | 0.0024 (7) | −0.0026 (6) |
| C8 | 0.0157 (9) | 0.0219 (9) | 0.0166 (8) | −0.0013 (7) | −0.0039 (7) | 0.0006 (7) |
| C9 | 0.0115 (8) | 0.0143 (8) | 0.0140 (8) | −0.0008 (7) | −0.0025 (6) | −0.0021 (6) |
| C10 | 0.0146 (9) | 0.0172 (8) | 0.0176 (8) | −0.0001 (7) | 0.0000 (7) | −0.0027 (7) |
| C11 | 0.0136 (8) | 0.0145 (8) | 0.0198 (8) | 0.0005 (7) | 0.0002 (7) | −0.0012 (7) |
| C12 | 0.0175 (9) | 0.0200 (9) | 0.0256 (9) | −0.0055 (7) | −0.0022 (8) | −0.0030 (8) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cu1—O1$^{i}$ | 1.9000 (11) | C5—C6 | 1.410 (2) |
| Cu1—O1 | 1.9000 (11) | C5—H5 | 0.9500 |
| Cu1—N1$^{i}$ | 2.0079 (13) | C6—C7 | 1.435 (2) |
| Cu1—N1 | 2.0079 (13) | C7—H7 | 0.9500 |
| N1—C7 | 1.293 (2) | C8—H8A | 0.9800 |
| N1—C9 | 1.474 (2) | C8—H8B | 0.9800 |
| O1—C1 | 1.3038 (19) | C8—H8C | 0.9800 |
| O2—C2 | 1.3724 (19) | C9—C10 | 1.522 (2) |
| O2—C8 | 1.4258 (19) | C9—H9A | 0.9900 |
| O3—C12 | 1.415 (2) | C9—H9B | 0.9900 |
| O3—C11 | 1.419 (2) | C10—C11 | 1.512 (2) |
| C1—C6 | 1.408 (2) | C10—H10A | 0.9900 |
| C1—C2 | 1.430 (2) | C10—H10B | 0.9900 |
| C2—C3 | 1.378 (2) | C11—H11A | 0.9900 |
| C3—C4 | 1.406 (2) | C11—H11B | 0.9900 |
| C3—H3 | 0.9500 | C12—H12A | 0.9800 |
| C4—C5 | 1.370 (2) | C12—H12B | 0.9800 |
| C4—H4 | 0.9500 | C12—H12C | 0.9800 |
| O1$^{i}$—Cu1—O1 | 180.0 | C6—C7—H7 | 115.9 |

| | | | |
|---|---|---|---|
| O1$^{i}$—Cu1—N1$^{i}$ | 92.11 (5) | O2—C8—H8A | 109.5 |
| O1—Cu1—N1$^{i}$ | 87.89 (5) | O2—C8—H8B | 109.5 |
| O1$^{i}$—Cu1—N1 | 87.89 (5) | H8A—C8—H8B | 109.5 |
| O1—Cu1—N1 | 92.11 (5) | O2—C8—H8C | 109.5 |
| N1$^{i}$—Cu1—N1 | 180.00 (7) | H8A—C8—H8C | 109.5 |
| C7—N1—C9 | 115.41 (14) | H8B—C8—H8C | 109.5 |
| C7—N1—Cu1 | 123.18 (11) | N1—C9—C10 | 111.16 (12) |
| C9—N1—Cu1 | 121.36 (10) | N1—C9—H9A | 109.4 |
| C1—O1—Cu1 | 129.66 (11) | C10—C9—H9A | 109.4 |
| C2—O2—C8 | 116.66 (13) | N1—C9—H9B | 109.4 |
| C12—O3—C11 | 112.53 (13) | C10—C9—H9B | 109.4 |
| O1—C1—C6 | 124.41 (15) | H9A—C9—H9B | 108.0 |
| O1—C1—C2 | 118.23 (14) | C11—C10—C9 | 111.67 (13) |
| C6—C1—C2 | 117.35 (14) | C11—C10—H10A | 109.3 |
| O2—C2—C3 | 124.78 (15) | C9—C10—H10A | 109.3 |
| O2—C2—C1 | 114.10 (14) | C11—C10—H10B | 109.3 |
| C3—C2—C1 | 121.12 (15) | C9—C10—H10B | 109.3 |
| C2—C3—C4 | 120.37 (15) | H10A—C10—H10B | 107.9 |
| C2—C3—H3 | 119.8 | O3—C11—C10 | 108.16 (14) |
| C4—C3—H3 | 119.8 | O3—C11—H11A | 110.1 |
| C5—C4—C3 | 119.73 (16) | C10—C11—H11A | 110.1 |
| C5—C4—H4 | 120.1 | O3—C11—H11B | 110.1 |
| C3—C4—H4 | 120.1 | C10—C11—H11B | 110.1 |
| C4—C5—C6 | 120.85 (16) | H11A—C11—H11B | 108.4 |
| C4—C5—H5 | 119.6 | O3—C12—H12A | 109.5 |
| C6—C5—H5 | 119.6 | O3—C12—H12B | 109.5 |
| C1—C6—C5 | 120.53 (15) | H12A—C12—H12B | 109.5 |
| C1—C6—C7 | 121.93 (15) | O3—C12—H12C | 109.5 |
| C5—C6—C7 | 117.53 (15) | H12A—C12—H12C | 109.5 |
| N1—C7—C6 | 128.21 (16) | H12B—C12—H12C | 109.5 |
| N1—C7—H7 | 115.9 | | |
| O1$^{i}$—Cu1—N1—C7 | −173.21 (13) | C3—C4—C5—C6 | −1.4 (2) |
| O1—Cu1—N1—C7 | 6.79 (13) | O1—C1—C6—C5 | −179.61 (15) |
| O1$^{i}$—Cu1—N1—C9 | 4.07 (11) | C2—C1—C6—C5 | 1.5 (2) |
| O1—Cu1—N1—C9 | −175.93 (11) | O1—C1—C6—C7 | 1.2 (3) |
| N1$^{i}$—Cu1—O1—C1 | 172.75 (14) | C2—C1—C6—C7 | −177.67 (14) |
| N1—Cu1—O1—C1 | −7.25 (14) | C4—C5—C6—C1 | 0.4 (2) |
| Cu1—O1—C1—C6 | 4.5 (2) | C4—C5—C6—C7 | 179.60 (14) |
| Cu1—O1—C1—C2 | −176.60 (10) | C9—N1—C7—C6 | 178.39 (15) |
| C8—O2—C2—C3 | 0.2 (2) | Cu1—N1—C7—C6 | −4.2 (2) |
| C8—O2—C2—C1 | 179.96 (13) | C1—C6—C7—N1 | −1.1 (3) |
| O1—C1—C2—O2 | −1.3 (2) | C5—C6—C7—N1 | 179.74 (16) |
| C6—C1—C2—O2 | 177.71 (13) | C7—N1—C9—C10 | −101.17 (16) |
| O1—C1—C2—C3 | 178.53 (14) | Cu1—N1—C9—C10 | 81.35 (15) |
| C6—C1—C2—C3 | −2.5 (2) | N1—C9—C10—C11 | 172.66 (13) |
| O2—C2—C3—C4 | −178.62 (14) | C12—O3—C11—C10 | −177.34 (13) |
| C1—C2—C3—C4 | 1.6 (2) | C9—C10—C11—O3 | −64.55 (18) |

| | |
|---|---|
| C2—C3—C4—C5 | 0.4 (2) |

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8B···O3$^{ii}$ | 0.98 | 2.58 | 3.476 (2) | 151 |
| C9—H9A···O1$^{i}$ | 0.99 | 2.31 | 2.782 (2) | 108 |
| C9—H9B···O3 | 0.99 | 2.55 | 2.918 (2) | 102 |

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

**Fig. 1**

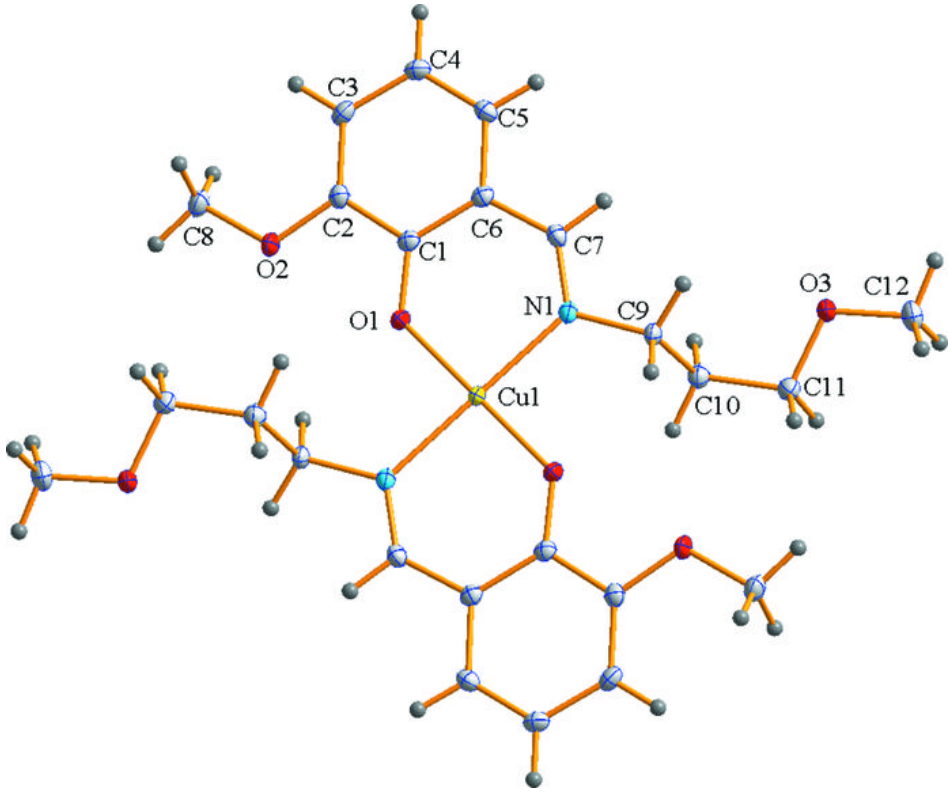

**Fig. 2**