Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

trans-Bis[(*S*)-2-(4-ethyl-4,5-dihydro-1,3-oxazol-2-yl)phenolato-κ^2N,O]copper(II)

Yan Zhang,[a] Tian-Fu Liu,[a]* Wen-Guo Xu,[a] Bang-Tun Zhao[b] and Jian-Ge Wang[b]

[a]Institute for Chemical Physics and Department of Chemistry, Beijing Institute of Technology, Beijing 100081, People's Republic of China, and [b]Department of Chemistry, Luoyang Normal University, Luoyang 471022, People's Republic of China
Correspondence e-mail: liutf@bit.edu.cn

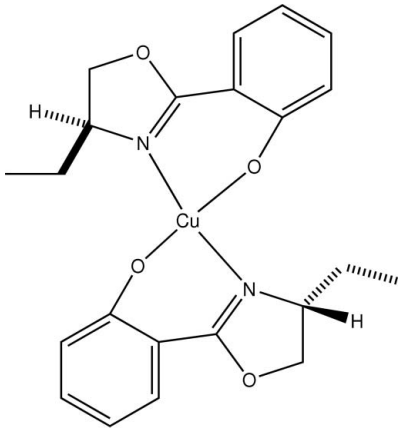
Received 17 March 2007; accepted 1 August 2007

Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.026; wR factor = 0.077; data-to-parameter ratio = 14.0.

In the title centrosymmetric compound, $[Cu(C_{11}H_{12}NO_2)_2]$, the coordination geometry of the Cu^{II} atom, which is on an inversion centre, is distorted square planar, with a Cu—N distance of 1.9541 (14) and a Cu—O distance of 1.9083 (14) Å. The crystal packing is stabilized by π–π interactions, with a centroid-to-centroid distance of 3.7953 (12) Å, and by C—H$\cdots\pi$ interactions.

Related literature

For related literature, see Chelucci (1997); Du *et al.* (2003); Ghosh *et al.* (1998); Ji *et al.* (1999); Imai *et al.* (1996); Zhang *et al.* (2007). For synthesis, see: Serrano *et al.* (1995).



Experimental

Crystal data

$[Cu(C_{11}H_{12}NO_2)_2]$
M_r = 443.97
Monoclinic, $P2_1/c$
a = 6.6645 (9) Å
b = 14.5796 (19) Å
c = 10.5615 (14) Å
β = 95.163 (1)°
V = 1022.1 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.10 mm^{-1}
T = 291 (2) K
0.48 × 0.27 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.621, T_{max} = 0.821
6062 measured reflections
1882 independent reflections
1652 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.077
S = 1.08
1882 reflections
134 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.9083 (14)	Cu1—N1	1.9541 (14)
O1^i—Cu1—O1	180	O1—Cu1—N1^i	89.19 (6)
O1—Cu1—N1	90.81 (6)		

Symmetry code: (i) $-x, -y+1, -z+1$.

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

Cg is the centroid of the benzene ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C9—H9$A\cdots Cg^{ii}$	0.97	2.89	3.632 (2)	134
C9—H9$A\cdots Cg^{iii}$	0.97	2.94	3.814 (2)	151

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

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); 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, 1999); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

The authors acknowledge support from the Natural Science Foundation Council of China (NSFC) (grant No. 20401003) and the Excellent Young Scholars Research Fund of Beijing Institute of Technology (grant No. 000Y07-26).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RN2023).

References

Bruker (1999). *SHELXTL*. Version 6.14. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chelucci, G. (1997). *Tetrahedron Asymmetry*, **8**, 2667–2670.
Du, D. M., Fu, B. F. & Hua, W. T. (2003). *Tetrahedron*, **59**, 1933–1938.
Ghosh, A. K., Mathivanan, P. & Cappiello, J. (1998). *Tetrahedron Asymmetry*, **9**, 1–45.

  doi:10.1107/S1600536807037919

Imai, Y., Zhang, W. B., Kida, T., Nakatsuji, Y. & Ikeda, I. (1996). *Tetrahedron Asymmetry*, **7**, 2453–2462.
Ji, J., Barnes, D. M., Zhang, J., King, S. A., Wittenberger, S. J. & Morton, H. E. (1999). *J. Am. Chem. Soc.* **121**, 10215–10216.
Serrano, J. L., Sierra, T., Gonzalez, Y., Bolm, C., Weickhardt, K., Magnus, A. & Moll, G. (1995). *J. Am. Chem. Soc.* **117**, 8312–8321.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Zhang, Y., Kong, D., Liu, T.-F. & Xu, W.-G. (2007). *Acta Cryst.* E**63**, m1396.

supplementary materials

Acta Cryst. (2007). E**63**, m2292-m2293 [**doi:10.1107/S1600536807037919**]

trans-Bis[(*S*)-2-(4-ethyl-4,5-dihydro-1,3-oxazol-2-yl)phenolato-κ^2N,O]copper(II)

Y. Zhang, T.-F. Liu, W.-G. Xu, B.-T. Zhao and J.-G. Wang

Comment

Over the last decade, C_2-symmetric chiral oxazoline metal complexes have been recognized as an effective class of chiral catalyst in a variety of transition metal catalyzed asymmetric reactions (Ghosh *et al.*, 1998). High catalytic activities and enantiomeric excesses have been obtained using C_2-symmetric chiral ligands in conjunction with suitable transition metal ion, for example, the hydrosilylation of ketone (Imai *et al.*, 1996), allylic alkylation (Chelucci 1997), Michael addition (Ji *et al.*, 1999), Diels-Alder cycloaddition, and cyclopropanation. Thus, the design and synthesis of new chiral oxazoline ligands and their complexes have inspired many scientists to work with great efforts (Du *et al.*, 2003; Zhang *et al.*, 2007).

We report here the crystal structure of the title compound, (I), a Cu^{II} complex with the chiral (*S*)-2-(4-ethyl-4,5-dihydrooxazol −2-yl)phenol, as the coordination ligand.

The title compound, contains one centrosymmetric tetra-coordinated copper(II) complex (Fig 1). The copper atom is coordinated by two 2-(4-ethyl- 4,5-dihydrooxazol-2-yl)-phenol anions, which bind to the metal centre *via* the N atom and the phenolyl O atom. Pairs of equivalent ligands lie *trans* to each other in a slightly distorted square planar geometry about the copper(II) atom (see Table 1).

The aryl and oxazoline least-squares planes are linked by π-π stacking interactions with Cg-Cg^{ii} distances 3.7953 (12) Å (symmetry code ii: $1-x, 1-y, 1-z$). The C—H···Cg (aryl ring) interactions are observed with H9A^{iii}···Cg = 2.94 Å (symmetry code iii: $x, 1/2-y, -1/2+z$) and H9A^{i}···Cg = 2.89 Å (Fig 2) (Spek, 2003).

Experimental

The chiral ligand, (*S*)-2-(4-ethyl-4,5-dihydrooxazol-2-yl)phenol was prepared from 2-hydroxybenzonitrile and (*S*)-2-aminobutan-1-ol as literature reported (Serrano *et al.*, 1995).

A solution of (*S*)-2-(4-ethyl-4,5-dihydrooxazol-2-yl)phenol (30.56 mg, 0.16 mmol) in methanol (1.60 ml) was added to a stirred solution of $CuCl_2 3H_2O$ (34.10 mg, 0.2 mmol) in methanol(2.00 ml). Crystals suitable for diffraction analysis were obtained after a few days.

Refinement

H atoms were positioned geometrically (aromatic C—H = 0.93 Å, aliphatic C—H = 0.96–0.98 Å) and refined with the riding model approximation, with U_{iso}(H) = 1.2U_{eq}(C) [1.5U_{eq}(C) for methyl H].

Figures

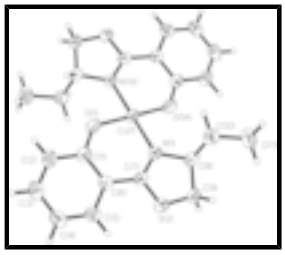


Fig. 1. *ORTEP* plot of $[Cu(C_{11}H_{12}NO_2)_2]$; displacement ellipsoids are drawn at the 30% probability level. (suffix A denotes symmetry code: $-x$, $-y$, $-z + 1$).

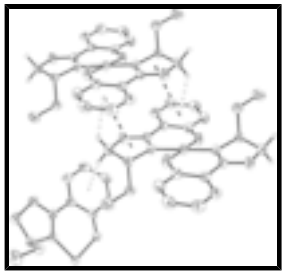


Fig. 2. The π–π stacking interactions and C—H···π interactions between ligands. Non-interaction hydrogen atoms are omitted for clarity.

trans-Bis[(_S_)-2-(4-ethyl-4,5-dihydro-1,3-oxazol-2-yl)phenolato- κ^2N,O]copper(II)

Crystal data

$[Cu(C_{11}H_{12}N_1O_2)_2]$	F_{000} = 462
M_r = 443.97	D_x = 1.443 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3198 reflections
a = 6.6645 (9) Å	θ = 2.4–26.7º
b = 14.5796 (19) Å	μ = 1.10 mm^{-1}
c = 10.5615 (14) Å	T = 291 (2) K
β = 95.1630 (10)º	Block, dark green
V = 1022.1 (2) Å^3	0.48 × 0.27 × 0.19 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	1882 independent reflections
Radiation source: fine-focus sealed tube	1652 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.013
Detector resolution: 0 pixels mm^{-1}	θ_{max} = 25.5º
T = 291(2) K	θ_{min} = 2.4º
φ and ω scans	h = −8→8
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	k = −17→17
T_{min} = 0.621, T_{max} = 0.821	l = −12→12
6062 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.026$	H-atom parameters constrained
$wR(F^2) = 0.077$	$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 0.1918P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
1882 reflections	$\Delta\rho_{max} = 0.19$ e Å^{-3}
134 parameters	$\Delta\rho_{min} = -0.19$ 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	0.0000	0.5000	0.5000	0.05203 (14)
O1	0.0943 (2)	0.53611 (12)	0.66862 (13)	0.0721 (4)
O2	0.5047 (2)	0.64456 (9)	0.42505 (13)	0.0618 (4)
N1	0.2068 (2)	0.57490 (10)	0.43014 (14)	0.0491 (3)
C1	0.2700 (3)	0.56981 (13)	0.71016 (18)	0.0552 (4)
C2	0.3213 (3)	0.57523 (15)	0.84174 (19)	0.0688 (5)
H2	0.2271	0.5573	0.8967	0.083*
C3	0.5071 (4)	0.60636 (15)	0.8920 (2)	0.0726 (6)
H3	0.5363	0.6089	0.9797	0.087*
C4	0.6509 (3)	0.63390 (15)	0.8124 (2)	0.0715 (6)
H4	0.7774	0.6534	0.8462	0.086*
C5	0.6042 (3)	0.63190 (14)	0.6845 (2)	0.0609 (5)
H5	0.6998	0.6513	0.6313	0.073*
C6	0.4154 (3)	0.60134 (12)	0.62996 (17)	0.0490 (4)
C7	0.3682 (3)	0.60446 (12)	0.49455 (17)	0.0487 (4)
C8	0.2135 (3)	0.60125 (12)	0.29532 (16)	0.0504 (4)
H8	0.1946	0.5468	0.2411	0.060*
C9	0.4282 (3)	0.63686 (15)	0.2930 (2)	0.0632 (5)
H9A	0.5091	0.5944	0.2485	0.076*
H9B	0.4289	0.6961	0.2512	0.076*
C10	0.0526 (3)	0.67215 (15)	0.2555 (2)	0.0665 (5)
H10A	−0.0764	0.6510	0.2799	0.080*
H10B	0.0848	0.7293	0.2998	0.080*
C11	0.0365 (4)	0.68926 (19)	0.1130 (2)	0.0902 (8)
H11A	0.1656	0.7075	0.0879	0.135*
H11B	−0.0600	0.7370	0.0920	0.135*
H11C	−0.0062	0.6340	0.0690	0.135*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0521 (2)	0.0579 (2)	0.0478 (2)	−0.01417 (13)	0.01397 (14)	−0.00670 (13)
O1	0.0673 (9)	0.0990 (11)	0.0521 (8)	−0.0319 (8)	0.0174 (7)	−0.0150 (8)
O2	0.0532 (7)	0.0665 (9)	0.0667 (9)	−0.0141 (6)	0.0114 (6)	0.0104 (7)
N1	0.0506 (8)	0.0491 (8)	0.0487 (8)	−0.0064 (6)	0.0097 (6)	−0.0020 (6)
C1	0.0607 (11)	0.0506 (10)	0.0548 (10)	−0.0062 (8)	0.0081 (8)	−0.0073 (8)
C2	0.0817 (14)	0.0709 (13)	0.0545 (11)	−0.0105 (11)	0.0097 (10)	−0.0077 (10)
C3	0.0901 (16)	0.0666 (13)	0.0580 (12)	−0.0029 (11)	−0.0105 (11)	−0.0065 (10)
C4	0.0680 (13)	0.0644 (13)	0.0779 (15)	−0.0036 (10)	−0.0173 (11)	−0.0024 (11)
C5	0.0542 (11)	0.0533 (11)	0.0742 (13)	−0.0025 (8)	0.0007 (9)	0.0033 (9)
C6	0.0515 (9)	0.0390 (9)	0.0564 (10)	0.0012 (7)	0.0041 (8)	−0.0013 (7)
C7	0.0489 (9)	0.0373 (9)	0.0613 (11)	0.0005 (7)	0.0132 (8)	0.0020 (7)
C8	0.0578 (10)	0.0462 (9)	0.0489 (9)	−0.0023 (8)	0.0141 (8)	−0.0009 (8)
C9	0.0633 (12)	0.0657 (12)	0.0623 (12)	−0.0030 (9)	0.0154 (9)	0.0145 (10)
C10	0.0670 (13)	0.0693 (13)	0.0634 (12)	0.0140 (10)	0.0076 (10)	−0.0008 (10)
C11	0.1026 (19)	0.0967 (19)	0.0690 (14)	0.0271 (15)	−0.0048 (13)	0.0096 (13)

Geometric parameters (Å, °)

Cu1—O1^{i}	1.9083 (14)	C4—H4	0.9300
Cu1—O1	1.9083 (14)	C5—C6	1.408 (3)
Cu1—N1	1.9541 (14)	C5—H5	0.9300
Cu1—N1^{i}	1.9541 (14)	C6—C7	1.437 (3)
O1—C1	1.309 (2)	C8—C10	1.521 (3)
O2—C7	1.352 (2)	C8—C9	1.524 (3)
O2—C9	1.446 (3)	C8—H8	0.9800
N1—C7	1.294 (2)	C9—H9A	0.9700
N1—C8	1.479 (2)	C9—H9B	0.9700
C1—C2	1.403 (3)	C10—C11	1.520 (3)
C1—C6	1.419 (3)	C10—H10A	0.9700
C2—C3	1.379 (3)	C10—H10B	0.9700
C2—H2	0.9300	C11—H11A	0.9600
C3—C4	1.390 (3)	C11—H11B	0.9600
C3—H3	0.9300	C11—H11C	0.9600
C4—C5	1.359 (3)		
O1^{i}—Cu1—O1	180	C1—C6—C7	120.29 (16)
O1^{i}—Cu1—N1	89.19 (6)	N1—C7—O2	115.27 (16)
O1—Cu1—N1	90.81 (6)	N1—C7—C6	127.55 (16)
O1^{i}—Cu1—N1^{i}	90.81 (6)	O2—C7—C6	117.16 (16)
O1—Cu1—N1^{i}	89.19 (6)	N1—C8—C10	111.15 (14)
N1—Cu1—N1^{i}	180	N1—C8—C9	102.36 (14)
C1—O1—Cu1	128.74 (12)	C10—C8—C9	113.79 (17)
C7—O2—C9	107.09 (14)	N1—C8—H8	109.8
C7—N1—C8	108.87 (14)	C10—C8—H8	109.8

C7—N1—Cu1	124.68 (12)	C9—C8—H8	109.8
C8—N1—Cu1	126.31 (11)	O2—C9—C8	105.14 (14)
O1—C1—C2	118.93 (18)	O2—C9—H9A	110.7
O1—C1—C6	124.03 (17)	C8—C9—H9A	110.7
C2—C1—C6	117.03 (18)	O2—C9—H9B	110.7
C3—C2—C1	122.0 (2)	C8—C9—H9B	110.7
C3—C2—H2	119.0	H9A—C9—H9B	108.8
C1—C2—H2	119.0	C11—C10—C8	111.75 (17)
C2—C3—C4	120.4 (2)	C11—C10—H10A	109.3
C2—C3—H3	119.8	C8—C10—H10A	109.3
C4—C3—H3	119.8	C11—C10—H10B	109.3
C5—C4—C3	119.1 (2)	C8—C10—H10B	109.3
C5—C4—H4	120.5	H10A—C10—H10B	107.9
C3—C4—H4	120.5	C10—C11—H11A	109.5
C4—C5—C6	122.0 (2)	C10—C11—H11B	109.5
C4—C5—H5	119.0	H11A—C11—H11B	109.5
C6—C5—H5	119.0	C10—C11—H11C	109.5
C5—C6—C1	119.43 (18)	H11A—C11—H11C	109.5
C5—C6—C7	120.26 (17)	H11B—C11—H11C	109.5
$O1^{i}$—Cu1—O1—C1	−70 (4)	C2—C1—C6—C7	−175.30 (18)
N1—Cu1—O1—C1	−20.2 (2)	C8—N1—C7—O2	−4.4 (2)
$N1^{i}$—Cu1—O1—C1	159.8 (2)	Cu1—N1—C7—O2	171.45 (11)
$O1^{i}$—Cu1—N1—C7	−161.26 (15)	C8—N1—C7—C6	173.99 (16)
O1—Cu1—N1—C7	18.74 (15)	Cu1—N1—C7—C6	−10.1 (3)
$N1^{i}$—Cu1—N1—C7	−143 (7)	C9—O2—C7—N1	−3.2 (2)
$O1^{i}$—Cu1—N1—C8	13.88 (15)	C9—O2—C7—C6	178.17 (16)
O1—Cu1—N1—C8	−166.12 (15)	C5—C6—C7—N1	176.24 (18)
$N1^{i}$—Cu1—N1—C8	32 (7)	C1—C6—C7—N1	−5.5 (3)
Cu1—O1—C1—C2	−167.87 (16)	C5—C6—C7—O2	−5.4 (3)
Cu1—O1—C1—C6	11.8 (3)	C1—C6—C7—O2	172.87 (16)
O1—C1—C2—C3	177.2 (2)	C7—N1—C8—C10	−112.28 (18)
C6—C1—C2—C3	−2.4 (3)	Cu1—N1—C8—C10	71.94 (19)
C1—C2—C3—C4	0.2 (4)	C7—N1—C8—C9	9.56 (19)
C2—C3—C4—C5	1.6 (3)	Cu1—N1—C8—C9	−166.22 (12)
C3—C4—C5—C6	−1.0 (3)	C7—O2—C9—C8	9.1 (2)
C4—C5—C6—C1	−1.3 (3)	N1—C8—C9—O2	−11.01 (19)
C4—C5—C6—C7	176.96 (18)	C10—C8—C9—O2	109.00 (18)
O1—C1—C6—C5	−176.67 (19)	N1—C8—C10—C11	−171.40 (18)
C2—C1—C6—C5	3.0 (3)	C9—C8—C10—C11	73.7 (2)
O1—C1—C6—C7	5.1 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9A···Cg^{ii}	0.97	2.89	3.632 (2)	134
C9—H9A···Cg^{iii}	0.97	2.94	3.814 (2)	151

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

Fig. 1

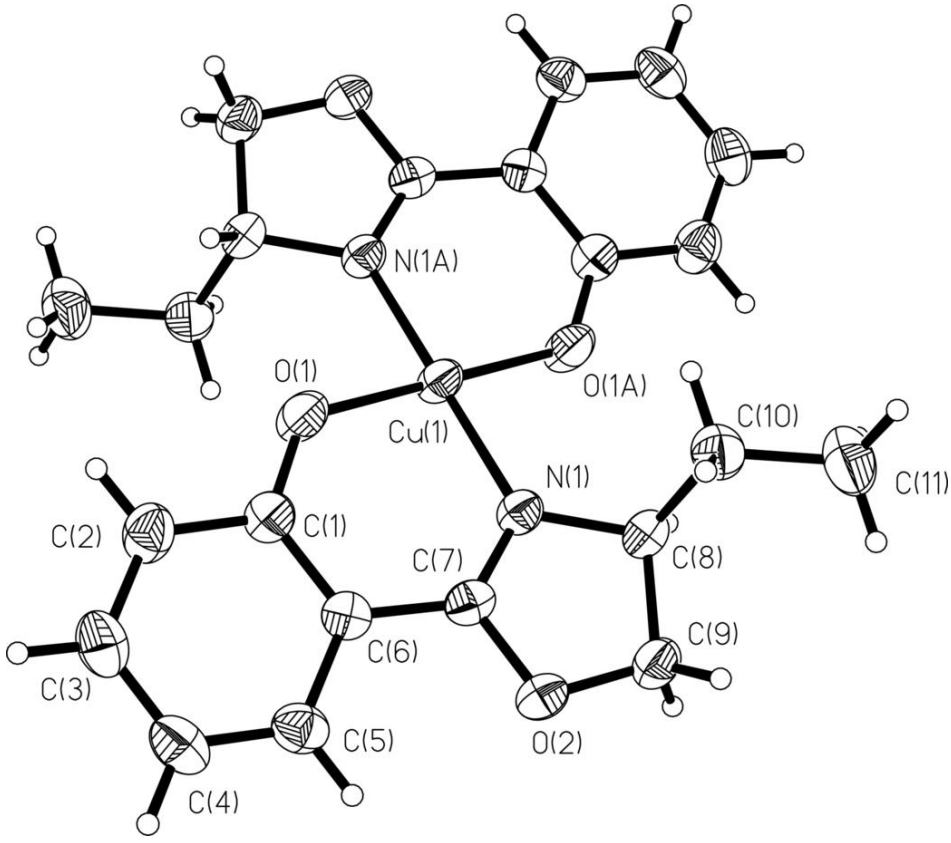


Fig. 2