Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetra-μ_2-acetato-$\kappa^8O:O'$-bis[(isoquinoline-κN)copper(II)]

Meng-Jiao Li, Jing-Jing Nie and Duan-Jun Xu*

Department of Chemistry, Zhejiang University, People's Republic of China
Correspondence e-mail: xudj@mail.hz.zj.cn

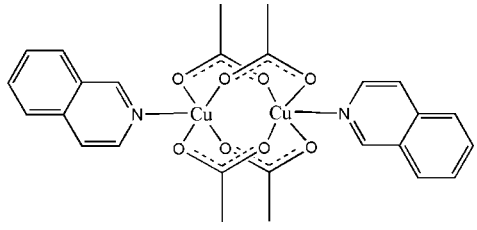
Received 2 July 2009; accepted 2 July 2009

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.025; wR factor = 0.074; data-to-parameter ratio = 17.4.

In the crystal structure of the title compound, $[Cu_2(CH_3COO)_4(C_9H_7N)_2]$, the Cu^{II} cation is coordinated by four acetate anions and one isoquinoline molecule in a distorted square-pyramidal geometry; the Cu^{II} cation is 0.1681 (6) Å from the basal coordination plane formed by the four O atoms. Each acetate anion bridges two Cu^{II} cations to form the centrosymmetric dinuclear complex. Within the dinuclear molecule, the Cu···Cu separation is 2.6459 (4) Å. A parallel arrangement of isoquinoline ligands of adjacent complexes is observed in the crystal structure; the face-to-face distance of 3.610 (10) Å suggests there is no π–π stacking between isoquinoline ring systems.

Related literature

For general background on the nature of π–π stacking, see: Su & Xu (2004); Xu *et al.* (2007). For related isoquinoline complexes, see: Clegg & Straughan (1989); Ivanikova *et al.* (2006). For a related quinoline complex, see: Pan & Xu (2004). For the metal atomic deviation from the basal coordination plane in square-pyramidal coordination geometry, see: Xie & Xu (2005). For the Cu···Cu distance in a polymeric Cu^{II} complex, see: Li *et al.* (2007).



Experimental

Crystal data

$[Cu_2(C_2H_3O_2)_4(C_9H_7N)_2]$ M_r = 621.57
Monoclinic, $P2_1/n$
a = 12.2278 (3) Å
b = 8.1610 (2) Å
c = 13.5309 (4) Å
β = 103.827 (8)°
V = 1311.13 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.67 mm^{-1}
T = 294 K
0.28 × 0.26 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.635, T_{max} = 0.720
12480 measured reflections
2997 independent reflections
2638 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.074
S = 1.06
2997 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu—N1	2.1789 (15)	Cu—O3	1.9777 (13)
Cu—O1	1.9771 (13)	Cu—O4^{i}	1.9740 (13)
Cu—O2^{i}	1.9728 (13)		

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This work was supported by the ZIJIN project of Zhejiang University, China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2151).

References

Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
Clegg, W. & Straughan, B. P. (1989). *Acta Cryst.* C**45**, 1992–1994.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Ivanikova, R., Boca, R., Dlhan, L., Fuess, H., Maslejova, A., Mrazova, V., Svoboda, I. & Titis, J. (2006). *Polyhedron*, **25**, 3261–3268.
Li, D.-X., Xu, D.-J. & Xu, Y.-Z. (2007). *J. Coord. Chem.* **60**, 2687–2694.
Pan, T.-T. & Xu, D.-J. (2004). *Acta Cryst.* E**60**, m56–m58.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Su, J.-R. & Xu, D.-J. (2004). *J. Coord. Chem.* **57**, 223–229.
Xie, A.-L. & Xu, D.-J. (2005). *J. Coord. Chem.* **58**, 225–230.
Xu, D.-J., Zhang, B.-Y., Su, J.-R. & Nie, J.-J. (2007). *Acta Cryst.* C**63**, m622–m624.

supplementary materials

Acta Cryst. (2009). E**65**, m881 [**doi:10.1107/S1600536809025732**]

Tetra-μ_2-acetato-$\kappa^8O:O'$-bis[(isoquinoline-κN)copper(II)]

M.-J. Li, J.-J. Nie and D.-J. Xu

Comment

As part of our ongoing investigation on the nature of π-π stacking (Su & Xu, 2004; Xu *et al.*, 2007), the title complex incorporating isoquinoline ligand has recently been prepared in the laboratory and its crystal structure is reported here.

The molecular structure is shown in Fig. 1. The Cu^{II} cation is coordinated by four O atoms from four acetate anions in the basal plane, an isoquinoline molecule coordinates to the Cu^{II} cation in the apical position to complete the distorted square-pyramidal coordination geometry. The Cu^{II} cation is 0.1681 (6) Å deviated from the basal coordination plane, which is consistent with the situation found in complexes with square-pyramidal coordination geometry (Xie & Xu, 2005). The Cu—N bond in the apical direction is longer than Cu—O bonds in the basal plane by *ca* 0.2 Å, showing the typical Jahn-Teller distortion. Each acetate anion bridges two Cu^{II} cations to form the centro-symmetric dinuclear complex. Within the dinuclear molecule the Cu···Cu separation is 2.6459 (4) Å, similar to 2.642 Å found in a polymeric Cu^{II} complex bridged by thiourea (Li *et al.* 2007).

The parallel arrangement of isoquinoline ligands of adjacent complexes is observed in the crystal structure (Fig. 2). The face-to-face distance of 3.610 (10) Å is close to 3.573 (5) Å found in a quinoline complex (Pan & Xu, 2004) and suggests no π-π stacking between isoquinoline ring systems.

Experimental

A water-ethanol solution (10 ml, 1:2) of isoquinoline (0.12 ml, 1 mmol) and copper acetate monohydrate (0.10 g, 0.5 mmol) was refluxed for 2.5 h. After cooling to room temperature the solution was filtered. The single crystals of the title compound were obtained from the filtrate after 3 d.

Refinement

Methyl H atoms were equally disordered over two sites with C—H = 0.96 Å, U_{iso}(H) = 1.5U_{eq}(C). Aromatic H atoms were placed in calculated positions with C—H = 0.93 Å and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C).

Figures

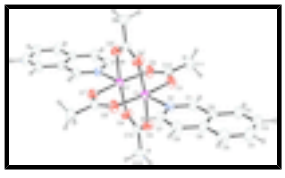


Fig. 1. The molecular structure of the title compound with 40% probability displacement (arbitrary spheres for H atoms). The disordered methyl H atoms are not shown for clarify [symmetry code: (i) 1 - *x*, 1 - *y*, 1 - *z*].

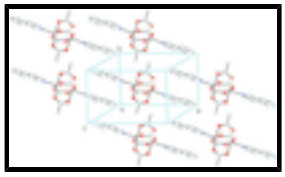


Fig. 2. The unit cell packing diagram showing the parallel arrangement of isoquinoline ligands.

Tetra-μ$_2$-acetato-κ^8*O*:*O*'-bis[(isoquinoline- κ*N*)copper(II)]

Crystal data

$[Cu_2(C_2H_3O_2)_4(C_9H_7N)_2]$	F_{000} = 636
M_r = 621.57	D_x = 1.574 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 10519 reflections
a = 12.2278 (3) Å	θ = 3.0–25.5º
b = 8.1610 (2) Å	μ = 1.67 mm^{-1}
c = 13.5309 (4) Å	T = 294 K
β = 103.827 (8)º	Chunk, blue
V = 1311.13 (7) Å^3	0.28 × 0.26 × 0.20 mm
Z = 2	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	2997 independent reflections
Radiation source: fine-focus sealed tube	2638 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.024
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 27.4º
T = 294 K	θ_{min} = 3.0º
ω scans	h = −15→15
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −10→10
T_{min} = 0.635, T_{max} = 0.720	l = −17→17
12480 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
$R[F^2 > 2\sigma(F^2)]$ = 0.025	H-atom parameters constrained
$wR(F^2)$ = 0.074	$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 0.4143P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.001
2997 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
172 parameters	$\Delta\rho_{min}$ = −0.40 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}	Occ. (<1)
Cu	0.411018 (16)	0.55776 (2)	0.528203 (14)	0.03074 (9)	
N1	0.26051 (12)	0.65641 (18)	0.56603 (11)	0.0360 (3)	
O1	0.32898 (12)	0.45444 (18)	0.39965 (11)	0.0457 (3)	
O2	0.47861 (11)	0.35876 (18)	0.35131 (10)	0.0453 (3)	
O3	0.43805 (12)	0.75437 (16)	0.45194 (11)	0.0451 (3)	
O4	0.58673 (12)	0.65621 (17)	0.40330 (11)	0.0457 (3)	
C1	0.16249 (15)	0.6461 (2)	0.49949 (14)	0.0378 (4)	
H1	0.1593	0.5883	0.4396	0.045*	
C2	−0.04146 (17)	0.7044 (3)	0.43993 (16)	0.0496 (5)	
H2	−0.0450	0.6483	0.3794	0.060*	
C3	−0.13598 (18)	0.7741 (3)	0.4580 (2)	0.0576 (6)	
H3	−0.2040	0.7653	0.4096	0.069*	
C4	−0.13180 (19)	0.8585 (3)	0.5482 (2)	0.0595 (6)	
H4	−0.1972	0.9052	0.5593	0.071*	
C5	−0.03322 (19)	0.8738 (3)	0.62062 (18)	0.0547 (5)	
H5	−0.0318	0.9312	0.6803	0.066*	
C6	0.17226 (17)	0.8114 (3)	0.67579 (15)	0.0476 (5)	
H6	0.1791	0.8668	0.7370	0.057*	
C7	0.26360 (16)	0.7388 (3)	0.65421 (14)	0.0428 (4)	
H7	0.3320	0.7457	0.7022	0.051*	
C8	0.06221 (15)	0.7172 (2)	0.51336 (14)	0.0364 (4)	
C9	0.06649 (16)	0.8026 (2)	0.60497 (14)	0.0395 (4)	
C10	0.37462 (16)	0.3780 (2)	0.34010 (13)	0.0365 (4)	
C11	0.2983 (2)	0.3021 (3)	0.24755 (17)	0.0588 (6)	
H11A	0.3428	0.2473	0.2081	0.088*	0.50
H11B	0.2540	0.3861	0.2071	0.088*	0.50
H11C	0.2493	0.2244	0.2685	0.088*	0.50
H11D	0.2213	0.3245	0.2477	0.088*	0.50
H11E	0.3101	0.1857	0.2487	0.088*	0.50
H11F	0.3148	0.3474	0.1873	0.088*	0.50
C12	0.51710 (15)	0.7661 (2)	0.40790 (13)	0.0361 (4)	

C13	0.5292 (2)	0.9275 (3)	0.3568 (2)	0.0589 (6)	
H13A	0.4710	1.0012	0.3656	0.088*	0.50
H13B	0.5226	0.9096	0.2855	0.088*	0.50
H13C	0.6015	0.9742	0.3869	0.088*	0.50
H13D	0.5924	0.9221	0.3264	0.088*	0.50
H13E	0.5408	1.0137	0.4065	0.088*	0.50
H13F	0.4619	0.9491	0.3051	0.088*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.02788 (12)	0.03427 (13)	0.03091 (13)	0.00155 (8)	0.00869 (8)	−0.00023 (8)
N1	0.0332 (7)	0.0399 (8)	0.0368 (7)	0.0025 (6)	0.0117 (6)	0.0014 (6)
O1	0.0362 (7)	0.0574 (9)	0.0413 (7)	−0.0006 (6)	0.0050 (6)	−0.0134 (6)
O2	0.0393 (7)	0.0568 (9)	0.0388 (7)	0.0013 (6)	0.0074 (5)	−0.0118 (6)
O3	0.0476 (8)	0.0401 (7)	0.0518 (8)	0.0056 (6)	0.0203 (6)	0.0090 (6)
O4	0.0450 (7)	0.0423 (7)	0.0554 (8)	0.0042 (6)	0.0231 (6)	0.0123 (6)
C1	0.0375 (9)	0.0428 (10)	0.0346 (9)	0.0026 (8)	0.0114 (7)	−0.0010 (7)
C2	0.0396 (10)	0.0552 (12)	0.0504 (11)	0.0017 (9)	0.0034 (9)	−0.0025 (9)
C3	0.0337 (10)	0.0629 (14)	0.0717 (15)	0.0037 (10)	0.0040 (10)	0.0051 (12)
C4	0.0389 (11)	0.0697 (15)	0.0745 (15)	0.0144 (11)	0.0224 (11)	0.0079 (12)
C5	0.0492 (12)	0.0660 (14)	0.0549 (12)	0.0133 (11)	0.0242 (10)	−0.0007 (11)
C6	0.0470 (11)	0.0602 (12)	0.0369 (9)	0.0062 (10)	0.0124 (8)	−0.0086 (9)
C7	0.0355 (9)	0.0547 (11)	0.0377 (9)	0.0015 (9)	0.0076 (7)	−0.0045 (8)
C8	0.0336 (9)	0.0371 (9)	0.0396 (9)	0.0004 (7)	0.0112 (7)	0.0056 (7)
C9	0.0376 (9)	0.0432 (10)	0.0408 (9)	0.0048 (8)	0.0152 (8)	0.0041 (8)
C10	0.0397 (9)	0.0368 (9)	0.0304 (8)	−0.0032 (8)	0.0032 (7)	0.0001 (7)
C11	0.0534 (13)	0.0723 (15)	0.0437 (11)	−0.0073 (11)	−0.0021 (9)	−0.0175 (11)
C12	0.0378 (9)	0.0343 (9)	0.0349 (8)	−0.0040 (8)	0.0059 (7)	0.0025 (7)
C13	0.0721 (16)	0.0412 (11)	0.0687 (15)	−0.0020 (10)	0.0271 (13)	0.0150 (10)

Geometric parameters (Å, °)

Cu—N1	2.1789 (15)	C4—H4	0.9300
Cu—O1	1.9771 (13)	C5—C9	1.412 (3)
Cu—O2^{i}	1.9728 (13)	C5—H5	0.9300
Cu—O3	1.9777 (13)	C6—C7	1.356 (3)
Cu—O4^{i}	1.9740 (13)	C6—C9	1.416 (3)
Cu—Cu^{i}	2.6459 (4)	C6—H6	0.9300
N1—C1	1.318 (2)	C7—H7	0.9300
N1—C7	1.362 (2)	C8—C9	1.412 (3)
O1—C10	1.251 (2)	C10—C11	1.505 (3)
O2—C10	1.254 (2)	C11—H11A	0.9600
O2—Cu^{i}	1.9728 (13)	C11—H11B	0.9600
O3—C12	1.255 (2)	C11—H11C	0.9600
O4—C12	1.249 (2)	C11—H11D	0.9600
O4—Cu^{i}	1.9740 (13)	C11—H11E	0.9600
C1—C8	1.409 (3)	C11—H11F	0.9600

C1—H1	0.9300	C12—C13	1.510 (3)
C2—C3	1.362 (3)	C13—H13A	0.9600
C2—C8	1.415 (3)	C13—H13B	0.9600
C2—H2	0.9300	C13—H13C	0.9600
C3—C4	1.391 (3)	C13—H13D	0.9600
C3—H3	0.9300	C13—H13E	0.9600
C4—C5	1.366 (3)	C13—H13F	0.9600
$O2^{i}$—Cu—$O4^{i}$	89.28 (6)	O1—C10—O2	125.47 (17)
$O2^{i}$—Cu—O1	167.80 (6)	O1—C10—C11	117.25 (18)
$O4^{i}$—Cu—O1	89.03 (6)	O2—C10—C11	117.28 (18)
$O2^{i}$—Cu—O3	89.10 (6)	C10—C11—H11A	109.5
$O4^{i}$—Cu—O3	167.77 (6)	C10—C11—H11B	109.5
O1—Cu—O3	90.00 (6)	H11A—C11—H11B	109.5
$O2^{i}$—Cu—N1	97.34 (6)	C10—C11—H11C	109.5
$O4^{i}$—Cu—N1	97.72 (6)	H11A—C11—H11C	109.5
O1—Cu—N1	94.86 (6)	H11B—C11—H11C	109.5
O3—Cu—N1	94.51 (6)	C10—C11—H11D	109.5
$O2^{i}$—Cu—Cu^{i}	85.07 (4)	H11A—C11—H11D	141.1
$O4^{i}$—Cu—Cu^{i}	84.27 (4)	H11B—C11—H11D	56.3
O1—Cu—Cu^{i}	82.74 (4)	H11C—C11—H11D	56.3
O3—Cu—Cu^{i}	83.51 (4)	C10—C11—H11E	109.5
N1—Cu—Cu^{i}	176.88 (4)	H11A—C11—H11E	56.3
C1—N1—C7	117.39 (16)	H11B—C11—H11E	141.1
C1—N1—Cu	119.81 (12)	H11C—C11—H11E	56.3
C7—N1—Cu	122.68 (12)	H11D—C11—H11E	109.5
C10—O1—Cu	124.66 (12)	C10—C11—H11F	109.5
C10—O2—Cu^{i}	122.03 (12)	H11A—C11—H11F	56.3
C12—O3—Cu	123.63 (12)	H11B—C11—H11F	56.3
C12—O4—Cu^{i}	123.05 (12)	H11C—C11—H11F	141.1
N1—C1—C8	124.11 (17)	H11D—C11—H11F	109.5
N1—C1—H1	117.9	H11E—C11—H11F	109.5
C8—C1—H1	117.9	O4—C12—O3	125.49 (17)
C3—C2—C8	119.9 (2)	O4—C12—C13	117.46 (18)
C3—C2—H2	120.0	O3—C12—C13	117.04 (18)
C8—C2—H2	120.0	C12—C13—H13A	109.5
C2—C3—C4	120.6 (2)	C12—C13—H13B	109.5
C2—C3—H3	119.7	H13A—C13—H13B	109.5
C4—C3—H3	119.7	C12—C13—H13C	109.5
C5—C4—C3	121.1 (2)	H13A—C13—H13C	109.5
C5—C4—H4	119.5	H13B—C13—H13C	109.5
C3—C4—H4	119.5	C12—C13—H13D	109.5
C4—C5—C9	120.0 (2)	H13A—C13—H13D	141.1
C4—C5—H5	120.0	H13B—C13—H13D	56.3
C9—C5—H5	120.0	H13C—C13—H13D	56.3
C7—C6—C9	119.90 (18)	C12—C13—H13E	109.5
C7—C6—H6	120.1	H13A—C13—H13E	56.3

C9—C6—H6	120.1	H13B—C13—H13E	141.1
C6—C7—N1	123.52 (17)	H13C—C13—H13E	56.3
C6—C7—H7	118.2	H13D—C13—H13E	109.5
N1—C7—H7	118.2	C12—C13—H13F	109.5
C1—C8—C9	117.99 (16)	H13A—C13—H13F	56.3
C1—C8—C2	122.54 (17)	H13B—C13—H13F	56.3
C9—C8—C2	119.46 (17)	H13C—C13—H13F	141.1
C8—C9—C5	118.87 (18)	H13D—C13—H13F	109.5
C8—C9—C6	117.09 (17)	H13E—C13—H13F	109.5
C5—C9—C6	124.04 (19)		

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

Fig. 1

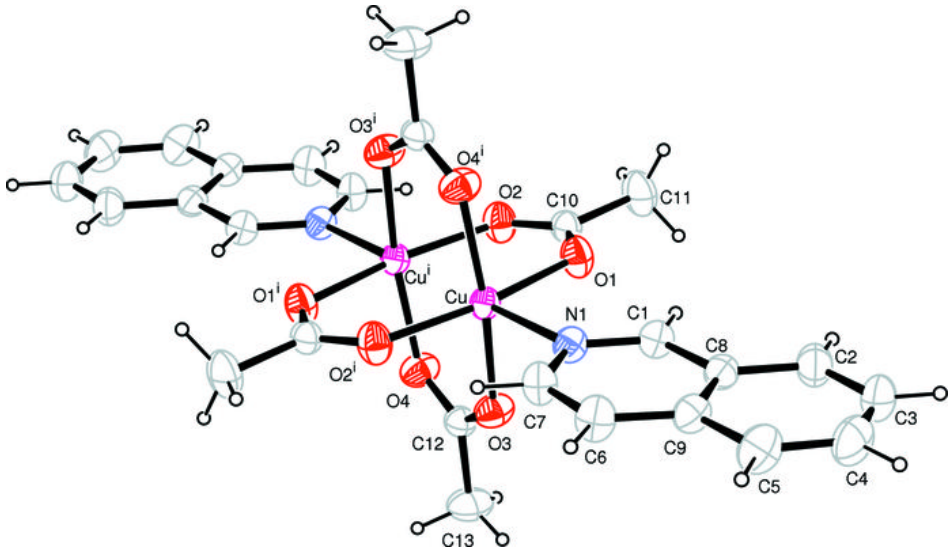

O3i
O4i
O2
C10
C11
Cui
O1
O1i
Cu
N1
C1
C8
C2
O2i
O4
C7
C3
C12
O3
C6
C9
C5
C4
C13

Fig. 2