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Tetra-μ-acetato-$\kappa^8O:O'$-bis[(4-vinylpyridine-κN)copper(II)](*Cu—Cu*)

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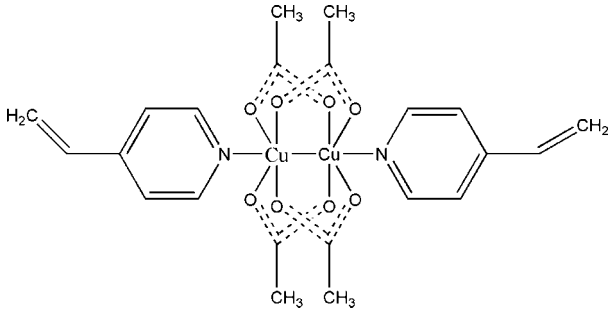
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.012 Å; R factor = 0.061; wR factor = 0.182; data-to-parameter ratio = 16.4.

The title compound, $[Cu_2(C_2H_3O_2)_4(C_7H_7N)_2]$, consists of centrosymmetric dinuclear units, in which four acetate groups bridge the two Cu atoms and a 4-vinylpyridine neutral ligand occupies the axial position of each Cu atom, coordinated to it through the pyridine N atom. Each Cu atom has a distorted octahedral coordination. Weak C—H···O interactions contribute to the crystal packing stability.

Related literature

For related literature, see: Seco *et al.* (2002).



Experimental

Crystal data

$C_{22}H_{26}Cu_2N_2O_8$
M_r = 573.53
Monoclinic, $P2_1/c$
a = 10.696 (2) Å
b = 12.830 (3) Å
c = 9.4820 (19) Å
β = 105.65 (3)°
V = 1253.0 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.74 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.623, T_{max} = 0.845
2455 measured reflections
2358 independent reflections
1830 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.182
S = 1.01
2358 reflections
144 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.47 e Å^{-3}
$\Delta\rho_{min}$ = −1.13 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—O2	1.969 (4)	Cu—O1	1.979 (4)
Cu—O3	1.971 (4)	Cu—N	2.178 (5)
Cu—O4	1.977 (5)	Cu—Cu^{i}	2.6405 (14)
O2—Cu—O3	89.4 (2)	O1—Cu—N	100.41 (19)
O3—Cu—O4	167.5 (2)	O2—Cu—Cu^{i}	81.48 (13)
O3—Cu—O1	88.7 (2)	O3—Cu—Cu^{i}	85.37 (14)
O4—Cu—O1	89.7 (2)	O4—Cu—Cu^{i}	82.19 (15)
O2—Cu—N	92.43 (19)	O1—Cu—Cu^{i}	85.69 (13)
O3—Cu—N	97.14 (19)	N—Cu—Cu^{i}	173.42 (15)
O4—Cu—N	95.30 (19)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···O2	0.93	2.54	3.083 (8)	118

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2001); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2001) and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2288).

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supplementary materials

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Tetra-μ-acetato-$\kappa^8O:O'$-bis[(4-vinylpyridine-κN)copper(II)](*Cu*-*Cu*)

F.-Q. Liu, R.-X. Li, S.-X. Li, L.-S. Sun and G.-Y. Liu

Comment

The title compound,(I), (Fig. 1), consists of centrosymmetric dinuclear units, in which four acetate groups bridge the two copper atoms and a 4-vinylpyridine neutral ligand occupies the axis position of each copper atom, coordinated to them through the pyridine nitrogen atom. Each copper atom has a distorted square-planar pyramidal coordination, with four oxygen atoms in a plane. The distances for Cu—O1, O2, O3 and O4 are 1.979 (4), 1.969 (4), 1.971 (4) and 1.977 (5) Å, respectively. The fifth coordination position is occupied by the pyridine nitrogen, N, of a ligand molecule at 2.178 (5) Å. All these values agree well with those observed in $[Cu_2(\upsilon\text{-}OOCCH_3)_4(PhNHpy)_2]$ (PhNHpy is 2-anilinopyridine) (Seco *et al.*, 2002). The copper atom rises from the basal plane to the apical N atom by 0.217 (1) Å. The Cu···Cu separation is 2.6405 (14) Å. Weak intramolecular C—H···O interactions contribute to the crystal packing stability.

Experimental

A solution of 4-vinylpyridine (1.05 g, 10 mmol) in alcohol (10 ml) was added to $Cu(OAc)_2{\cdot}H_2O$ (2.00 g, 10 mmol) in alcohol (40 ml). The solution was stirred during 2 h and a precipitate was formed. The blue precipitate was filtered off, washed with alcohol and dried *in vacuo* over $CaCO_3$. Blue crystals were obtained from recrystallization in alcohol after a few days.

Refinement

H atoms were positioned geometrically (C—H = 0.93 Å or 0.96 Å) and allowed to ride on their parent atoms with U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C).

Figures

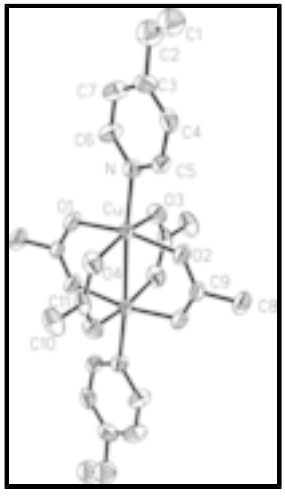

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme, hydrogen atoms were omitted for clarity.

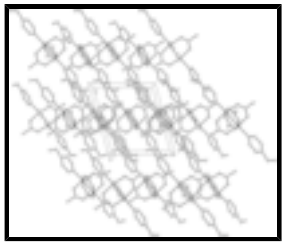

Fig. 2. The packing of (I), viewed down the *b* axis.

Tetra-μ-acetato-κ^8*O*:*O*'-bis[(4-vinylpyridine-κ*N*)copper(II)](Cu—Cu)

Crystal data

$C_{22}H_{26}Cu_2N_2O_8$	F_{000} = 588
M_r = 573.53	D_x = 1.520 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3329 reflections
a = 10.696 (2) Å	θ = 2.5–25.1º
b = 12.830 (3) Å	μ = 1.74 mm^{-1}
c = 9.4820 (19) Å	T = 293 (2) K
β = 105.65 (3)º	Block, blue
V = 1253.0 (5) Å^3	0.30 × 0.20 × 0.10 mm
Z = 2	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	2358 independent reflections
Radiation source: fine-focus sealed tube	1830 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.013
T = 293(2) K	θ_{max} = 26.0º
thin–slice ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	h = −13→12
T_{min} = 0.623, T_{max} = 0.845	k = 0→15
2455 measured reflections	l = 0→11

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.061	H-atom parameters constrained
$wR(F^2)$ = 0.182	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 3P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.002
2358 reflections	$\Delta\rho_{max}$ = 1.47 e Å^{-3}

144 parameters	$\Delta\rho_{min} = -1.13$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
Cu	0.40251 (7)	0.02266 (5)	0.05538 (7)	0.0441 (3)
O1	0.3606 (5)	−0.1277 (3)	0.0336 (5)	0.0612 (11)
O2	0.4745 (5)	0.1639 (3)	0.0554 (5)	0.0630 (12)
O3	0.3013 (5)	0.0430 (4)	−0.1496 (5)	0.0641 (12)
O4	0.5344 (5)	−0.0066 (4)	0.2417 (5)	0.0663 (12)
N	0.2542 (5)	0.0760 (4)	0.1573 (5)	0.0508 (11)
C1	−0.0518 (10)	0.2562 (8)	0.4014 (10)	0.101
H1A	0.0269	0.2911	0.4345	0.121*
H1B	−0.1233	0.2774	0.4321	0.121*
C2	−0.0617 (10)	0.1780 (8)	0.3125 (10)	0.100
H2A	−0.1386	0.1412	0.2771	0.120*
C3	0.0585 (7)	0.1517 (7)	0.2715 (8)	0.074 (2)
C4	0.1672 (8)	0.2085 (5)	0.2806 (8)	0.0677 (19)
H4A	0.1774	0.2736	0.3251	0.081*
C5	0.2638 (6)	0.1679 (5)	0.2221 (7)	0.0562 (15)
H5A	0.3382	0.2073	0.2293	0.067*
C6	0.1465 (7)	0.0221 (6)	0.1532 (8)	0.0691 (19)
H6A	0.1387	−0.0437	0.1106	0.083*
C7	0.0486 (8)	0.0551 (8)	0.2057 (9)	0.083 (2)
H7A	−0.0243	0.0136	0.1978	0.099*
C8	0.6099 (8)	0.3033 (6)	0.0297 (10)	0.082 (2)
H8A	0.5859	0.3336	0.1111	0.123*
H8B	0.5659	0.3391	−0.0587	0.123*
H8C	0.7020	0.3093	0.0448	0.123*
C9	0.5718 (6)	0.1895 (5)	0.0165 (7)	0.0501 (14)
C10	0.7308 (8)	−0.0547 (7)	0.4061 (7)	0.080 (2)
H10A	0.8105	−0.0162	0.4246	0.121*
H10B	0.7496	−0.1279	0.4161	0.121*
H10C	0.6842	−0.0343	0.4752	0.121*

C11	0.6490 (7)	−0.0322 (4)	0.2527 (7)	0.0563 (16)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.0535 (4)	0.0386 (4)	0.0448 (4)	0.0010 (3)	0.0212 (3)	0.0026 (3)
O1	0.076 (3)	0.044 (2)	0.074 (3)	−0.012 (2)	0.038 (2)	0.001 (2)
O2	0.073 (3)	0.042 (2)	0.085 (3)	−0.007 (2)	0.041 (3)	0.000 (2)
O3	0.066 (3)	0.073 (3)	0.051 (2)	0.012 (2)	0.011 (2)	0.004 (2)
O4	0.085 (3)	0.069 (3)	0.045 (2)	0.011 (3)	0.017 (2)	0.004 (2)
N	0.054 (3)	0.052 (3)	0.049 (3)	0.000 (2)	0.019 (2)	−0.001 (2)
C1	0.101	0.101	0.101	0.000	0.027	0.000
C2	0.100	0.100	0.100	0.000	0.027	0.000
C3	0.067 (4)	0.107 (7)	0.058 (4)	0.029 (4)	0.034 (3)	0.028 (4)
C4	0.099 (5)	0.048 (4)	0.068 (4)	0.020 (4)	0.043 (4)	0.010 (3)
C5	0.061 (4)	0.053 (4)	0.063 (4)	0.000 (3)	0.030 (3)	0.008 (3)
C6	0.064 (4)	0.074 (5)	0.077 (5)	−0.020 (4)	0.033 (4)	−0.018 (4)
C7	0.066 (4)	0.103 (7)	0.091 (6)	−0.009 (4)	0.043 (4)	−0.003 (5)
C8	0.089 (5)	0.047 (4)	0.120 (7)	−0.016 (4)	0.047 (5)	0.002 (4)
C9	0.061 (4)	0.039 (3)	0.056 (3)	−0.004 (3)	0.024 (3)	0.007 (3)
C10	0.104 (6)	0.073 (5)	0.051 (4)	0.021 (4)	−0.002 (4)	−0.001 (3)
C11	0.083 (5)	0.034 (3)	0.046 (3)	0.006 (3)	0.006 (3)	−0.001 (2)

Geometric parameters (Å, °)

Cu—O2	1.969 (4)	C3—C7	1.379 (12)
Cu—O3	1.971 (4)	C4—C5	1.399 (9)
Cu—O4	1.977 (5)	C4—H4A	0.9300
Cu—O1	1.979 (4)	C5—H5A	0.9300
Cu—N	2.178 (5)	C6—C7	1.343 (10)
Cu—Cu^{i}	2.6405 (14)	C6—H6A	0.9300
O1—C9^{i}	1.251 (7)	C7—H7A	0.9300
O2—C9	1.238 (7)	C8—C9	1.511 (9)
O3—C11^{i}	1.240 (8)	C8—H8A	0.9600
O4—C11	1.246 (9)	C8—H8B	0.9600
N—C5	1.320 (8)	C8—H8C	0.9600
N—C6	1.335 (8)	C9—O1^{i}	1.251 (7)
C1—C2	1.296 (8)	C10—C11	1.509 (8)
C1—H1A	0.9300	C10—H10A	0.9600
C1—H1B	0.9300	C10—H10B	0.9600
C2—C3	1.479 (12)	C10—H10C	0.9600
C2—H2A	0.9300	C11—O3^{i}	1.240 (8)
C3—C4	1.355 (11)		
O2—Cu—O3	89.4 (2)	C3—C4—C5	119.2 (7)
O2—Cu—O4	89.4 (2)	C3—C4—H4A	120.4
O3—Cu—O4	167.5 (2)	C5—C4—H4A	120.4
O2—Cu—O1	167.15 (17)	N—C5—C4	122.9 (6)
O3—Cu—O1	88.7 (2)	N—C5—H5A	118.5

O4—Cu—O1	89.7 (2)	C4—C5—H5A	118.5
O2—Cu—N	92.43 (19)	N—C6—C7	125.4 (8)
O3—Cu—N	97.14 (19)	N—C6—H6A	117.3
O4—Cu—N	95.30 (19)	C7—C6—H6A	117.3
O1—Cu—N	100.41 (19)	C6—C7—C3	118.6 (8)
O2—Cu—Cu^{i}	81.48 (13)	C6—C7—H7A	120.7
O3—Cu—Cu^{i}	85.37 (14)	C3—C7—H7A	120.7
O4—Cu—Cu^{i}	82.19 (15)	C9—C8—H8A	109.5
O1—Cu—Cu^{i}	85.69 (13)	C9—C8—H8B	109.5
N—Cu—Cu^{i}	173.42 (15)	H8A—C8—H8B	109.5
C9^{i}—O1—Cu	121.3 (4)	C9—C8—H8C	109.5
C9—O2—Cu	127.2 (4)	H8A—C8—H8C	109.5
C11^{i}—O3—Cu	121.6 (4)	H8B—C8—H8C	109.5
C11—O4—Cu	125.0 (4)	O2—C9—O1^{i}	124.3 (6)
C5—N—C6	115.7 (6)	O2—C9—C8	117.5 (6)
C5—N—Cu	120.8 (4)	O1^{i}—C9—C8	118.2 (6)
C6—N—Cu	123.4 (5)	C11—C10—H10A	109.5
C2—C1—H1A	120.0	C11—C10—H10B	109.5
C2—C1—H1B	120.0	H10A—C10—H10B	109.5
H1A—C1—H1B	120.0	C11—C10—H10C	109.5
C1—C2—C3	115.1 (10)	H10A—C10—H10C	109.5
C1—C2—H2A	122.5	H10B—C10—H10C	109.5
C3—C2—H2A	122.5	O3^{i}—C11—O4	125.8 (6)
C4—C3—C7	118.1 (7)	O3^{i}—C11—C10	118.6 (7)
C4—C3—C2	130.7 (9)	O4—C11—C10	115.6 (6)
C7—C3—C2	111.0 (8)		
O2—Cu—O1—C9^{i}	4.5 (12)	O4—Cu—N—C5	73.6 (5)
O3—Cu—O1—C9^{i}	86.0 (5)	O1—Cu—N—C5	164.3 (5)
O4—Cu—O1—C9^{i}	−81.6 (5)	O2—Cu—N—C6	160.8 (6)
N—Cu—O1—C9^{i}	−177.0 (5)	O3—Cu—N—C6	71.1 (6)
Cu^{i}—Cu—O1—C9^{i}	0.6 (5)	O4—Cu—N—C6	−109.6 (6)
O3—Cu—O2—C9	−87.1 (6)	O1—Cu—N—C6	−18.9 (6)
O4—Cu—O2—C9	80.5 (6)	C1—C2—C3—C4	−18.3 (14)
O1—Cu—O2—C9	−5.7 (12)	C1—C2—C3—C7	166.1 (9)
N—Cu—O2—C9	175.8 (5)	C7—C3—C4—C5	0.6 (11)
Cu^{i}—Cu—O2—C9	−1.7 (5)	C2—C3—C4—C5	−174.6 (7)
O2—Cu—O3—C11^{i}	80.3 (5)	C6—N—C5—C4	−1.4 (9)
O4—Cu—O3—C11^{i}	−4.3 (13)	Cu—N—C5—C4	175.7 (5)
O1—Cu—O3—C11^{i}	−87.0 (5)	C3—C4—C5—N	0.2 (10)
N—Cu—O3—C11^{i}	172.7 (5)	C5—N—C6—C7	1.8 (12)
Cu^{i}—Cu—O3—C11^{i}	−1.2 (5)	Cu—N—C6—C7	−175.2 (7)
O2—Cu—O4—C11	−81.0 (5)	N—C6—C7—C3	−1.0 (14)
O3—Cu—O4—C11	3.6 (13)	C4—C3—C7—C6	−0.3 (12)
O1—Cu—O4—C11	86.1 (5)	C2—C3—C7—C6	175.8 (8)

N—Cu—O4—C11	−173.4 (5)	Cu—O2—C9—O1^{i}	1.8 (10)
Cu^{i}—Cu—O4—C11	0.4 (5)	Cu—O2—C9—C8	−178.7 (5)
O2—Cu—N—C5	−16.0 (5)	Cu—O4—C11—O3^{i}	0.4 (10)
O3—Cu—N—C5	−105.7 (5)	Cu—O4—C11—C10	−177.7 (5)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5A···O2	0.93	2.54	3.083 (8)	118

Fig. 1

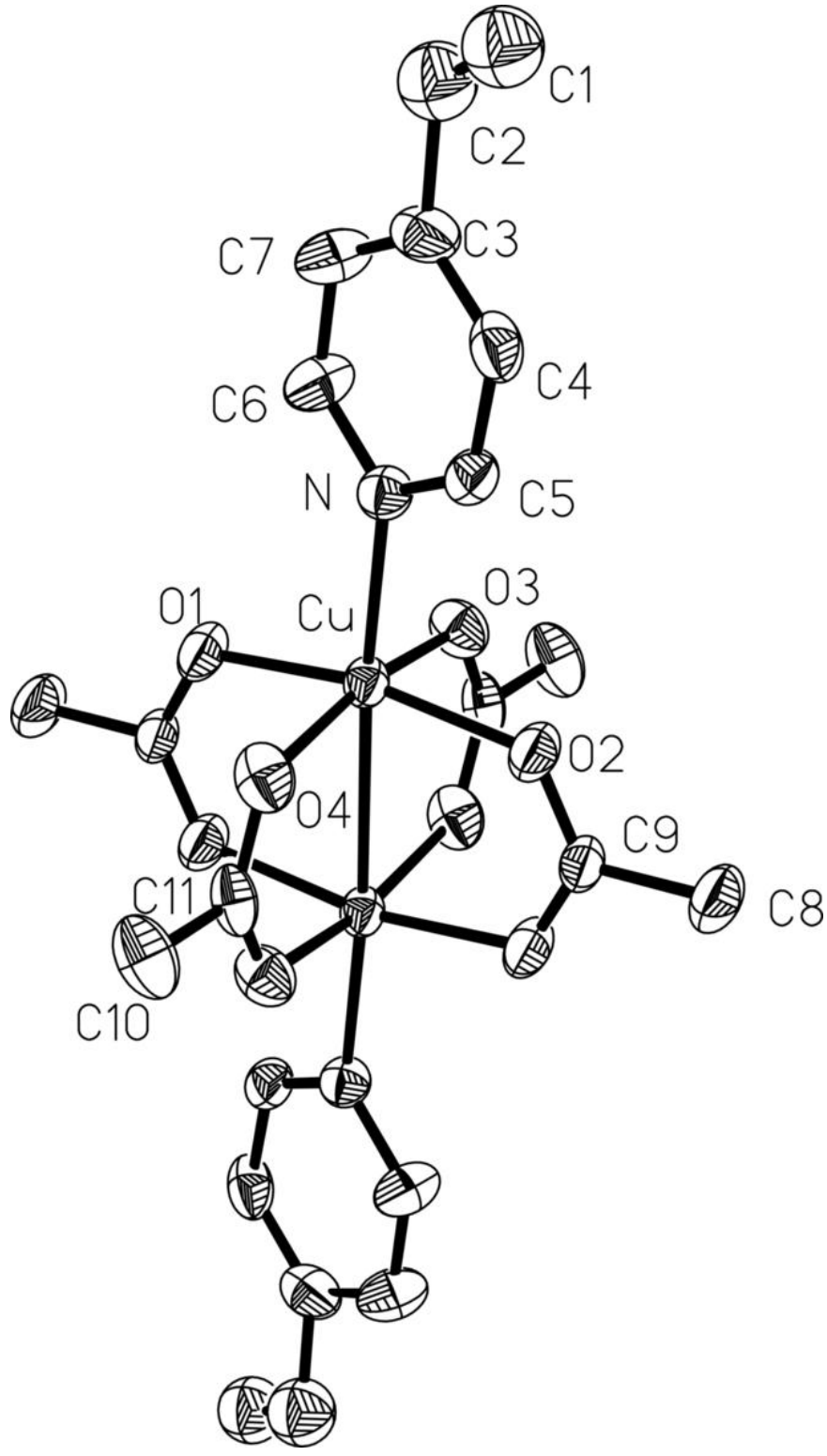

Fig. 2