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Bis{2-methoxy-6-[(3-pyridyl)methyliminomethyl]phenolato}copper(II)

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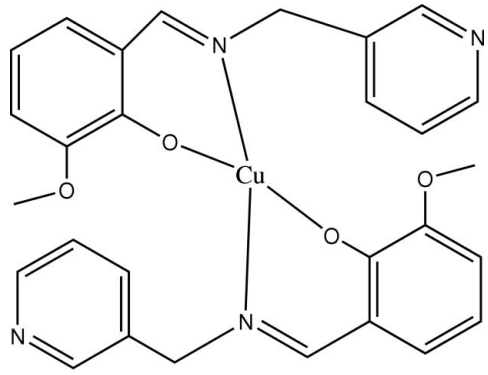
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.102; data-to-parameter ratio = 15.8.

In the mononuclear title complex, $[Cu(C_{14}H_{13}N_2O_2)_2]$, the Cu^{II} atom lies on an inversion centre and adopts a square-planar coordination geometry. The dihedral angle formed by the pyridine and benzene rings is 74.61 (5)°. Intramolecular C—H···O hydrogen bonds are present. The crystal structure is stabilized by weak aromatic π–π stacking interactions involving neighbouring pyridine rings [centroid–centroid distance = 3.853 (2) Å].

Related literature

For a related structure, see: Wang *et al.* (2008). For the synthetic procedure, see: Kannappan *et al.* (2005); Zhao *et al.* (2008).



Experimental

Crystal data

$[Cu(C_{14}H_{13}N_2O_2)_2]$
M_r = 546.07
Monoclinic, $P2_1/c$
a = 11.455 (2) Å
b = 14.414 (3) Å
c = 7.5491 (15) Å
β = 102.55 (3)°
V = 1216.7 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.94 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.824, T_{max} = 0.828
11771 measured reflections
2667 independent reflections
2430 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.102
S = 1.41
2667 reflections
169 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9B···O2^{i}	0.97	2.28	2.862 (2)	118

Symmetry code: (i) $-x+2, -y+2, -z$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL/PC*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2354).

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supplementary materials

Acta Cryst. (2009). E**65**, m1058 [**doi:10.1107/S1600536809029523**]

Bis{2-methoxy-6-[(3-pyridyl)methyliminomethyl]phenolato}copper(II)

Y. Wang, L.-L. Zhu and B.-W. Sun

Comment

Schiff base metal complexes have been frequently investigated in the past several years, because of their broad range of properties and applications. We herein report the crystal structure of a new complex formed by reaction of $Cu(CH_3COO)_2$ and the Schiff base ligand *N*-(3-pyridylmethyl)-3-methoxy-salicylaldiminato.

As shown in Fig. 1, the mononuclear title complex is centrosymmetric. The copper atom adopts a square planar coordination geometry provided by two *trans*-arranged phenolate-O and two imine-N atoms from two ligands (Wang *et al.*, 2008). The dihedral angle formed by the pyridine and benzene rings of the same ligand is 74.61 (5)°. An intramolecular C—H···O hydrogen bond (Table 1) stabilizes the molecular conformation. In the crystal structure, weak aromatic π–π stacking interactions involving neighbouring pyridine rings at (x, y, z) and (x, 5/2-y, 1/2+z) are present, with a centroid-to-centroid distance of 3.853 (2) Å.

Experimental

All chemicals were of reagent grade and were used as received with out further purification. 2-Hydroxy-3-methoxybenzaldehyde (0.152 g, 1 mmol) in ethanol (5 ml) was added to a stirred ethanol solution (5 ml) containing 3-aminomethylpyridine (0.108 g, 1 mmol). The resulting yellow solution was continuously stirred for about 1 h, then $Cu(CH_3COO)_2.H_2O$ (0.100 g, 0.5 mmol) in ethanol (5 ml) was added. The resulting deep green solution was stirred for another 2 h and left to evaporate at room temperature (Kannappan *et al.*,2005; Zhao *et al.*, 2008). After several days, dark green block crystals suitable for X-ray diffraction analysis were formed.

Refinement

All H atoms were located geometrically and treated as riding atoms, with C—H = 0.93–0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$ for methyl H atoms.

Figures

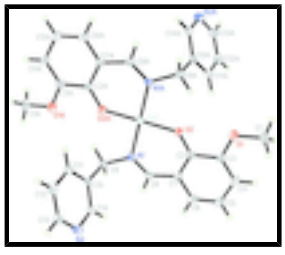

Fig. 1. The molecular structure of the title compound with the atom-numbering scheme and all hydrogen atoms. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code A: 2 - *x*, -*y*, 1 - *z*]

Bis{2-methoxy-6-[(3-pyridyl)methyliminomethyl]phenolato}copper(II)

Crystal data

$[Cu(C_{14}H_{13}N_2O_2)_2]$	$F(000) = 566$
$M_r = 546.07$	$D_x = 1.491$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 10382 reflections
$a = 11.455$ (2) Å	$\theta = 3.2–27.5°$
$b = 14.414$ (3) Å	$\mu = 0.94$ mm^{-1}
$c = 7.5491$ (15) Å	$T = 293$ K
$\beta = 102.55$ (3)°	Block, dark green
$V = 1216.7$ (4) Å^3	0.20 × 0.20 × 0.20 mm
$Z = 2$	

Data collection

Rigaku SCXmini diffractometer	2667 independent reflections
Radiation source: fine-focus sealed tube	2430 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.035$
Detector resolution: 13.6612 pixels mm^{-1}	$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
ω scans	$h = -14\rightarrow14$
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)	$k = -18\rightarrow18$
$T_{min} = 0.824$, $T_{max} = 0.828$	$l = -9\rightarrow9$
11771 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.035$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.102$	H-atom parameters constrained
$S = 1.41$	$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
2667 reflections	$(\Delta/\sigma)_{max} = 0.001$
169 parameters	$\Delta\rho_{max} = 0.25$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.62$ e Å^{-3}

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	1.0000	1.0000	0.0000	0.03101 (13)
N1	0.94828 (11)	1.08186 (9)	−0.22373 (17)	0.0269 (3)
C14	1.04327 (16)	1.27619 (11)	−0.3538 (2)	0.0346 (4)
H14A	0.9670	1.2747	−0.4280	0.041*
C9	1.02998 (15)	1.10214 (10)	−0.3470 (2)	0.0307 (4)
H9A	0.9841	1.1069	−0.4708	0.037*
H9B	1.0867	1.0517	−0.3417	0.037*
C11	1.20928 (16)	1.19482 (12)	−0.1813 (2)	0.0359 (4)
H11A	1.2487	1.1403	−0.1375	0.043*
C7	0.74950 (13)	1.11896 (10)	−0.1721 (2)	0.0294 (4)
O1	0.67391 (12)	1.03058 (10)	0.23920 (19)	0.0457 (3)
C8	0.84437 (15)	1.11952 (11)	−0.2697 (2)	0.0308 (4)
H8A	0.8285	1.1511	−0.3798	0.037*
C10	1.09654 (14)	1.19174 (11)	−0.2930 (2)	0.0284 (3)
N2	1.09381 (14)	1.35872 (10)	−0.3131 (2)	0.0413 (4)
C3	0.65892 (13)	1.07713 (11)	0.0778 (2)	0.0315 (4)
C6	0.64554 (16)	1.17021 (12)	−0.2470 (3)	0.0380 (4)
H6A	0.6412	1.2022	−0.3552	0.046*
C4	0.55774 (15)	1.12611 (12)	0.0004 (3)	0.0379 (4)
H4A	0.4931	1.1278	0.0566	0.045*
C13	1.20181 (17)	1.35935 (13)	−0.2044 (3)	0.0416 (4)
H13A	1.2384	1.4164	−0.1730	0.050*
C5	0.55195 (16)	1.17370 (13)	−0.1642 (3)	0.0424 (5)
H5A	0.4839	1.2075	−0.2160	0.051*
C1	0.58255 (19)	1.03860 (17)	0.3375 (3)	0.0501 (5)
H1A	0.6037	1.0030	0.4473	0.075*
H1B	0.5088	1.0157	0.2651	0.075*
H1C	0.5731	1.1026	0.3670	0.075*
C12	1.26288 (17)	1.28035 (13)	−0.1354 (3)	0.0426 (4)
H12A	1.3385	1.2843	−0.0595	0.051*
O2	0.85152 (11)	1.02297 (9)	0.07153 (19)	0.0383 (3)
C2	0.75880 (13)	1.07128 (10)	−0.0065 (2)	0.0287 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02621 (19)	0.03057 (19)	0.0384 (2)	0.00818 (10)	0.01174 (14)	0.01467 (11)

N1	0.0288 (7)	0.0212 (6)	0.0311 (7)	−0.0008 (5)	0.0075 (6)	0.0041 (5)
C14	0.0332 (9)	0.0296 (8)	0.0420 (9)	0.0005 (7)	0.0106 (7)	0.0065 (7)
C9	0.0374 (8)	0.0259 (8)	0.0310 (8)	0.0015 (7)	0.0123 (7)	0.0027 (6)
C11	0.0352 (9)	0.0339 (9)	0.0398 (10)	0.0047 (7)	0.0110 (8)	0.0057 (7)
C7	0.0267 (8)	0.0229 (7)	0.0368 (9)	0.0024 (6)	0.0028 (7)	0.0022 (6)
O1	0.0404 (8)	0.0547 (8)	0.0475 (8)	0.0114 (7)	0.0217 (7)	0.0147 (7)
C8	0.0350 (9)	0.0236 (8)	0.0326 (8)	−0.0014 (6)	0.0045 (7)	0.0069 (6)
C10	0.0329 (8)	0.0273 (8)	0.0290 (8)	0.0006 (6)	0.0155 (7)	0.0042 (6)
N2	0.0434 (9)	0.0280 (7)	0.0529 (10)	−0.0011 (6)	0.0119 (8)	0.0028 (7)
C3	0.0287 (8)	0.0272 (8)	0.0388 (9)	0.0008 (6)	0.0076 (7)	−0.0020 (7)
C6	0.0384 (9)	0.0342 (9)	0.0377 (9)	0.0084 (7)	0.0001 (8)	0.0054 (7)
C4	0.0291 (9)	0.0381 (9)	0.0466 (10)	0.0035 (7)	0.0085 (8)	−0.0074 (8)
C13	0.0438 (11)	0.0318 (9)	0.0498 (11)	−0.0056 (8)	0.0116 (9)	−0.0027 (8)
C5	0.0311 (9)	0.0437 (10)	0.0480 (11)	0.0134 (8)	−0.0014 (8)	0.0001 (8)
C1	0.0476 (12)	0.0642 (13)	0.0443 (11)	0.0038 (10)	0.0229 (10)	−0.0025 (10)
C12	0.0336 (9)	0.0505 (11)	0.0433 (10)	−0.0040 (8)	0.0074 (8)	−0.0022 (8)
O2	0.0295 (7)	0.0430 (6)	0.0452 (7)	0.0136 (5)	0.0144 (6)	0.0194 (6)
C2	0.0264 (8)	0.0213 (7)	0.0375 (9)	0.0016 (6)	0.0051 (7)	0.0017 (6)

Geometric parameters (Å, °)

Cu1—O2^{i}	1.9218 (13)	O1—C3	1.369 (2)
Cu1—O2	1.9218 (13)	O1—C1	1.413 (2)
Cu1—N1	2.0399 (13)	C8—H8A	0.9300
Cu1—N1^{i}	2.0399 (13)	N2—C13	1.328 (2)
N1—C8	1.285 (2)	C3—C4	1.374 (2)
N1—C9	1.485 (2)	C3—C2	1.427 (2)
C14—N2	1.329 (2)	C6—C5	1.354 (3)
C14—C10	1.394 (2)	C6—H6A	0.9300
C14—H14A	0.9300	C4—C5	1.408 (3)
C9—C10	1.510 (2)	C4—H4A	0.9300
C9—H9A	0.9700	C13—C12	1.378 (3)
C9—H9B	0.9700	C13—H13A	0.9300
C11—C10	1.381 (2)	C5—H5A	0.9300
C11—C12	1.387 (2)	C1—H1A	0.9600
C11—H11A	0.9300	C1—H1B	0.9600
C7—C6	1.411 (2)	C1—H1C	0.9600
C7—C2	1.411 (2)	C12—H12A	0.9300
C7—C8	1.439 (2)	O2—C2	1.2993 (18)
O2^{i}—Cu1—O2	180.0	C14—C10—C9	119.92 (15)
O2^{i}—Cu1—N1	89.00 (6)	C13—N2—C14	116.70 (16)
O2—Cu1—N1	91.00 (6)	O1—C3—C4	124.16 (16)
O2^{i}—Cu1—N1^{i}	91.00 (6)	O1—C3—C2	114.21 (14)
O2—Cu1—N1^{i}	89.00 (6)	C4—C3—C2	121.63 (16)
N1—Cu1—N1^{i}	180.00 (6)	C5—C6—C7	121.24 (17)
C8—N1—C9	114.85 (13)	C5—C6—H6A	119.4
C8—N1—Cu1	123.58 (12)	C7—C6—H6A	119.4

C9—N1—Cu1	121.57 (10)	C3—C4—C5	119.95 (17)
N2—C14—C10	124.60 (17)	C3—C4—H4A	120.0
N2—C14—H14A	117.7	C5—C4—H4A	120.0
C10—C14—H14A	117.7	N2—C13—C12	123.81 (17)
N1—C9—C10	110.44 (12)	N2—C13—H13A	118.1
N1—C9—H9A	109.6	C12—C13—H13A	118.1
C10—C9—H9A	109.6	C6—C5—C4	119.92 (16)
N1—C9—H9B	109.6	C6—C5—H5A	120.0
C10—C9—H9B	109.6	C4—C5—H5A	120.0
H9A—C9—H9B	108.1	O1—C1—H1A	109.5
C10—C11—C12	119.04 (16)	O1—C1—H1B	109.5
C10—C11—H11A	120.5	H1A—C1—H1B	109.5
C12—C11—H11A	120.5	O1—C1—H1C	109.5
C6—C7—C2	120.31 (16)	H1A—C1—H1C	109.5
C6—C7—C8	117.23 (15)	H1B—C1—H1C	109.5
C2—C7—C8	122.44 (14)	C13—C12—C11	118.62 (17)
C3—O1—C1	117.61 (15)	C13—C12—H12A	120.7
N1—C8—C7	128.12 (15)	C11—C12—H12A	120.7
N1—C8—H8A	115.9	C2—O2—Cu1	130.63 (12)
C7—C8—H8A	115.9	O2—C2—C7	124.05 (15)
C11—C10—C14	117.21 (15)	O2—C2—C3	119.02 (15)
C11—C10—C9	122.86 (14)	C7—C2—C3	116.93 (14)
$O2^{i}$—Cu1—N1—C8	175.74 (14)	C8—C7—C6—C5	−179.88 (16)
O2—Cu1—N1—C8	−4.26 (14)	O1—C3—C4—C5	178.43 (17)
$O2^{i}$—Cu1—N1—C9	−4.15 (11)	C2—C3—C4—C5	−1.4 (3)
O2—Cu1—N1—C9	175.85 (11)	C14—N2—C13—C12	0.8 (3)
C8—N1—C9—C10	86.53 (17)	C7—C6—C5—C4	0.4 (3)
Cu1—N1—C9—C10	−93.57 (13)	C3—C4—C5—C6	0.8 (3)
C9—N1—C8—C7	−174.86 (15)	N2—C13—C12—C11	0.0 (3)
Cu1—N1—C8—C7	5.3 (2)	C10—C11—C12—C13	−0.5 (3)
C6—C7—C8—N1	176.48 (16)	N1—Cu1—O2—C2	1.65 (16)
C2—C7—C8—N1	−2.3 (3)	$N1^{i}$—Cu1—O2—C2	−178.35 (16)
C12—C11—C10—C14	0.2 (3)	Cu1—O2—C2—C7	0.5 (3)
C12—C11—C10—C9	−178.60 (16)	Cu1—O2—C2—C3	−179.78 (12)
N2—C14—C10—C11	0.7 (3)	C6—C7—C2—O2	−179.72 (16)
N2—C14—C10—C9	179.51 (16)	C8—C7—C2—O2	−1.0 (3)
N1—C9—C10—C11	94.88 (18)	C6—C7—C2—C3	0.5 (2)
N1—C9—C10—C14	−83.88 (18)	C8—C7—C2—C3	179.25 (14)
C10—C14—N2—C13	−1.1 (3)	O1—C3—C2—O2	1.1 (2)
C1—O1—C3—C4	−4.3 (3)	C4—C3—C2—O2	−179.07 (16)
C1—O1—C3—C2	175.52 (16)	O1—C3—C2—C7	−179.13 (14)
C2—C7—C6—C5	−1.1 (3)	C4—C3—C2—C7	0.7 (2)

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9B···$O2^{i}$	0.97	2.28	2.862 (2)	118

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*.

Fig. 1