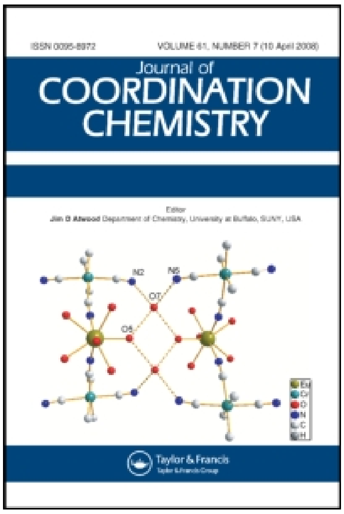

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Note: Synthesis And Crystal Structure Of Dipyridine-(Salicylidene-1-α-Aminobenzyl-2-Naphthol) Copper (II) Complex

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Note

SYNTHESIS AND CRYSTAL STRUCTURE OF DIPYRIDINE-(SALICYLIDENE-1-α-AMINOBENZYL-2-NAPHTHOL) COPPER (II) COMPLEX

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Keywords: Schiff base; Copper; Crystal structure

Transition metal complexes of tridentate Schiff bases have been of considerable interests in terms of structural chemistry and biological function [1]. In this note, we report the synthesis and crystal structure of the title complex Cu(L)(py)$_2$.

EXPERIMENTAL

Preparation of the Ligand and its Cu(II) Complex

The ligand (L) was synthesized by condensation of salicylaldehyde and 1-α-aminobenzyl-2-naphthol [2] which was prepared according to a method described in the literature [3,4]. To 1.25 g (5.0 mmol) of 1-α-aminobenzyl-2-naphthol in 20 cm^3 of ethanol, 0.73 g (6.0 mmol) of salicylaldehyde in 20 cm^3 of ethanol was added. The reaction mixture was stirred at room temperature overnight. The yellow precipitate formed was collected by filtration and washed with ethanol and ether. Pale yellow single crystals were obtained by slow evaporation of a CH_3CN solution of the compound. Elemental analysis: Calc. for $C_{24}H_{19}NO_2$(%): C, 81.49; H, 5.38; N, 3.96. Found: C, 81.26; H, 5.53; N, 3.81.

An ethanol solution of $Cu(ClO_4)_2 \cdot 6H_2O$ (0.186 g, 0.50 mmol, 20 cm^3) was added dropwise to 0.177 g (0.50 mmol) of the ligand in 50 cm^3 of ethanol. The mixture was stirred at 60°C for 2 h and the dark green precipitate was collected by filtration.

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TABLE I Crystal and refinement data for the complex

Empirical Formula	$C_{34}H_{27}CuN_3O_2$
Formula Weight	537.13
Crystal System	Monoclinic
Space Group	$P2_1/n$
a(Å)	12.4930(12)
b(Å)	14.0257(13)
c(Å)	15.9002(16)
β(°)	105.057(10)
V(Å^3)	2787.3(5)
Z	4
Density (Mg/m^3, Calc.)	1.366
Final $R[I > 2\ \sigma(I)]$	$R1 = 0.0500$ $wR2 = 0.2181$

The solid was washed with ethanol and ether and dried over P_2O_5. Dark brown single crystals suitable for crystallographic analysis were obtained by slow evaporation of a pyridine solution of the complex. Elemental analysis: Calc. for $C_{34}H_{27}CuN_3O_2$(%): C, 71.19; H, 4.71; N, 7.33. Found: C, 71.23; H, 4.56; N, 7.31.

X-ray Structure Determination

A single crystal was mounted on a glass fibre and intensity data were collected on a Siemens P4 four-circle diffractrometer with graphite-monochromated MoKα radiation ($\lambda = 0.71073$ Å) using the $\theta/2\theta$ scan mode with variable scan speed of 4.0–60°/min in ω. Data were collected for Lorantz and polarization effects. The structure was solved by direct methods. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares techniques [5]. Hydrogen atoms were found in a different Fourier map and refined isotropically. All computations were carried out on a PC using the SHELX-PC program package [6]. Crystal data for the title complex are collected in Table I.

RESULTS AND DISCUSSION

An ORTEP representation of the title complex with the numbering scheme is shown in Fig. 1. Selected bond lengths and bond angles are listed in Table II. As shown in Fig. 1, Cu(II) is five-coordinated by two O atoms and one N atom from the ligand L and two N atoms from pyridine molecules, giving rise to a distorted square-pyramidal geometry. The N3 atom from pyridine lies in an axial direction, and N1, O1, O2 from L and N2 from pyridine are in the basal plane with an average plane deviation of 0.499 Å; O1 and N1 atoms are located under the mean basal plane. As usual, the Cu atom lifts by 0.203 Å from the mean plane towards N3 in the complex. The coordination of this tridentate ligand to Cu(II) forms two six-membered rings having common Cu–N and Cu–O bond lengths. The Cu1–N2 (py) bond distance is 2.099(3) Å, which is slightly longer than 1.989(3) Å of Cu1–N1 (L). The axial Cu1–N3 (py) distance of 2.278(4) Å is appreciably longer than Cu1–N2 (py) due to Jahn–Teller effects. Bond angles N3–Cu1–O1, N3–Cu1–O2 and N3–Cu1–N2 are close to 90°. The bond angle of N3–Cu1–N1, however, is 106.28(14)°, being significantly larger than the others. Steric crowding causes this effect. The naphthol ring in the complex has a mean

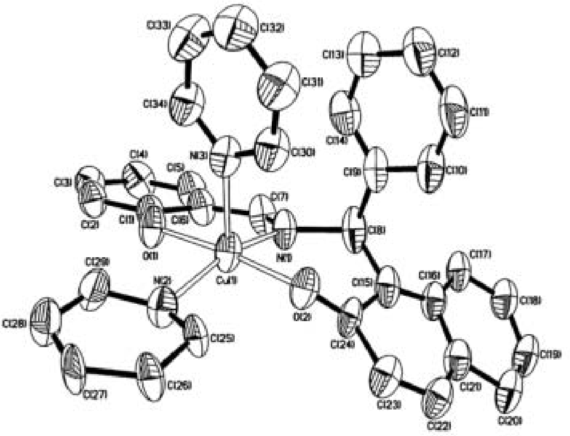

FIGURE 1 Molecular structure of the title complex showing 50% probability displacement ellipsoids.

TABLE II Selected bond lengths (Å) and bond angles (°) for the complex

Cu1–O1	1.921(2)	N1–Cu1–O1	92.19(12)
Cu1–O2	1.917(2)	N1–Cu1–O2	90.74(12)
Cu1–N1	1.989(3)	N1–Cu1–N2	162.04(15)
Cu1–N2	2.099(3)	N2–Cu1–O1	87.45(12)
Cu1–N3	2.278(4)	N2–Cu1–O2	88.05(12)
C1–O1	1.294(4)	N3–Cu1–O1	93.65(13)
C1–C2	1.415(5)	N3–Cu1–O2	91.08(13)
C1–C6	1.415(6)	N3–Cu1–N1	106.28(14)
N1–C7	1.280(5)	N3–Cu1–N2	91.66(13)
N1–C8	1.499(5)	O1–C1–C2	119.4(4)
O2–C24	1.319(9)	O1–C1–C6	123.8(3)
C15–C24	1.392(10)	O2–C24–C15	126(2)
C23–C24	1.407(10)	O2–C24–C23	123.9(18)
N2–C25	1.345(9)	C8–C9–C15	106.7(12)
N2–C29	1.355(8)	C15–C24–C23	105.9(16)
N3–C30	1.327(5)	C25–N2–C29	123.7(12)
N3–C34	1.312(6)	C30-N3–C34	116.7(5)
		Cu1–N2–C29	117.4(6)
		Cu1–N3–C30	119.3(4)
		Cu1–N3–C34	123.7(3)
		Cu1–O1–C1	128.9(2)

plane derivation of 0.255 Å, significantly larger than in the free ligand (0.04 Å). Bond distances and angles of the naphthyl ring in the complex are typical.

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Supplementary Data

Full lists of crystallographic data are available from the authors upon request.

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