Instrumental Achievements

Crystal Structure of (*N,N'*-Disalicylidene-2,3-diaminopyridine)copper(II) Complex

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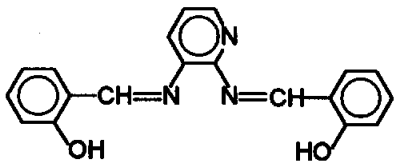
Behavior of *N,N'*-disalicylidene-2,3-diaminopyridine (**1**) against metal ions[1-3] and its X-ray structure[4] as well as its thermochromic and photochromic properties[5] have been reported. This communication presents the X-ray structure of Cu(II) complex (**2**) prepared by using ligand **1** (Fig. 1).

The ligand (5×10^{-4} mol, 0.1894 g) was dissolved in hot acetonitrile (100 ml) and a solution of $[Cu(CH_3COO)_2]\cdot H_2O$ (5×10^{-4} mol, 0.0998 g) in hot methanol (10 ml) was then added. The resulting solution was mixed and set aside for 24 h. The precipitated crystals were filtered and used for X-ray data collection with graphite-monochromatized Mo K_α radiation. The crystal and experimental data are presented in Table 1 and the



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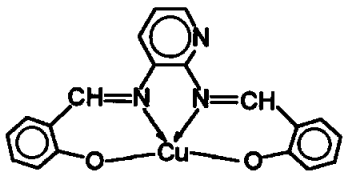

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Fig. 1 Chemical structures.

Table 1 Crystal and experimental data

Formula:	$C_{19}H_{13}CuN_3O_2$
Formula weight:	378.87
Crystal system:	monoclinic
Space group:	$P2_1/n$ $Z=4$
a	11.364(2) Å
b	7.817(3) Å
c	18.424(2) Å
β	107.369(4)°
V	1562.0(6) Å^3
D_x	1.611 g/cm^3
μ	1.4169 mm^{-1}
T	297 K
$F(0\,0\,0)$	772
Dark green	
Crystal size:	0.3×0.2×0.15 mm
R	0.058
Rw	0.059
No. of reflections used	1722
No. of parameters	226
Goodness-of-fit	0.84
Measurements:	Enraf-Nonius CAD-4 diffractometer
Program system:	CAD-4-EXPRESS Software
Structure determination:	MolEN
Treatment of hydrogen atoms:	geometric calculation
Refinement:	full-matrix least-squares (MolEN)

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Table 2 Final atomic coordinates and equivalent isotropic thermal parameters for non-hydrogen atoms

Atom	x	y	z	B_{eq}/Å^2
Cu	0.04755(9)	0.1663(1)	0.46150(5)	4.78(2)
O1	-0.1102(5)	0.2639(8)	0.4237(3)	5.5(1)
O2	0.0287(5)	0.0820(8)	0.3625(3)	5.7(1)
N1	0.0722(6)	0.2437(8)	0.5646(3)	5.1(2)
N2	0.2090(6)	0.0668(8)	0.5029(3)	5.0(2)
N3	0.3723(7)	0.039(1)	0.6206(4)	7.7(2)
C1	-0.1691(7)	0.351(1)	0.4615(4)	5.1(2)
C2	-0.2894(7)	0.407(1)	0.4230(5)	6.6(2)
C3	-0.3560(8)	0.504(1)	0.4583(5)	7.8(3)
C4	-0.3066(9)	0.551(1)	0.5347(5)	7.5(3)
C5	-0.1928(8)	0.500(1)	0.5740(5)	6.9(2)
C6	-0.1202(7)	0.398(1)	0.5401(4)	5.4(2)
C7	-0.0029(7)	0.342(1)	0.5859(4)	5.5(2)
C8	0.1855(7)	0.192(1)	0.6147(4)	5.3(2)
C9	0.2273(8)	0.228(1)	0.6909(4)	6.2(2)
C10	0.3427(9)	0.171(1)	0.7314(4)	8.2(3)
C11	0.4096(9)	0.080(1)	0.6954(5)	8.6(3)
C12	0.2600(7)	0.098(1)	0.5815(4)	5.4(2)
C13	0.2711(7)	-0.013(1)	0.4645(4)	5.5(2)
C14	0.2262(7)	-0.055(1)	0.3861(4)	5.3(2)
C15	0.3014(8)	-0.153(1)	0.3536(5)	7.2(2)
C16	0.2615(9)	-0.210(1)	0.2805(5)	7.9(3)
C17	0.1428(9)	-0.174(1)	0.2377(5)	8.1(3)
C18	0.0665(8)	-0.078(1)	0.2648(4)	6.7(2)
C19	0.1061(7)	-0.013(1)	0.3400(4)	5.1(2)

$B_{eq}=8\pi^2/3\Sigma_i\Sigma_j U_{ij}\,a_i^*a_j^*(a_i\cdot a_j)$.

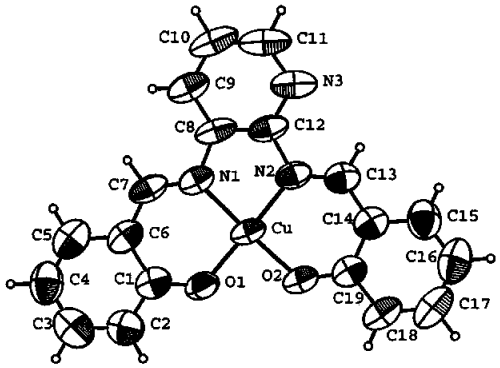

Fig. 2 The ORTEP plot of the title complex with atom labeling.

Table 3 Bond distances (Å) and angles (°)

Cu - O1	1.880(6)	C3 - C4	1.40(1)
Cu - O2	1.890(5)	C4 - C5	1.34(1)
Cu - N1	1.933(7)	C5 - C6	1.42(1)
Cu - N2	1.928(7)	C6 - C7	1.42(1)
O1 - C1	1.29(1)	C8 - C9	1.37(1)
O2 - C19	1.31(1)	C8 - C12	1.39(1)
N1 - C7	1.29(1)	C9 - C10	1.38(1)
N1 - C8	1.40(1)	C10 - C11	1.35(2)
N2 - C12	1.411(9)	C13 - C14	1.42(1)
N2 - C13	1.30(1)	C14 - C15	1.41(1)
N3 - C11	1.35(1)	C14 - C19	1.41(1)
N3 - C12	1.34(1)	C15 - C16	1.36(1)
C1 - C2	1.41(1)	C16 - C17	1.37(1)
C1 - C6	1.43(1)	C17 - C18	1.35(1)
C2 - C3	1.37(1)	C18 - C19	1.42(1)
O1 - Cu - O2	87.9(2)	C1 - C6 - C7	122.3(9)
O1 - Cu - N1	94.5(3)	C5 - C6 - C7	118.5(9)
O1 - Cu - N2	178.5(3)	N1 - C7 - C6	126.2(8)
O2 - Cu - N1	177.3(3)	N1 - C8 - C9	126(1)
O2 - Cu - N2	93.5(3)	N1 - C8 - C12	115.0(7)
N1 - Cu - N2	84.0(3)	C9 - C8 - C12	119.2(9)
Cu - O1 - C1	127.1(5)	C8 - C9 - C10	118(1)
Cu - O2 - C19	127.6(5)	C9 - C10 - C11	119.4(9)
Cu - N1 - C7	124.7(6)	N3 - C11 - C10	125(1)
Cu - N1 - C8	113.1(6)	N2 - C12 - N3	121.7(9)
C7 - N1 - C8	122.1(7)	N2 - C12 - C8	115.1(8)
Cu - N2 - C12	112.8(6)	N3 - C12 - C8	123.2(8)
Cu - N2 - C13	125.9(6)	N2 - C13 - C14	125.2(9)
C12 - N2 - C13	121.2(8)	C13 - C14 - C15	118.6(9)
C11 - N3 - C12	115(1)	C13 - C14 - C19	123.1(9)
O1 - C1 - C2	118.2(8)	C15 - C14 - C19	118.1(9)
O1 - C1 - C6	124.8(8)	C14 - C15 - C16	122(1)
C2 - C1 - C6	117.0(9)	C15 - C16 - C17	119(1)
C1 - C2 - C3	122(1)	C16 - C17 - C18	122(1)
C2 - C3 - C4	121(1)	C17 - C18 - C19	121(1)
C3 - C4 - C5	120(1)	O2 - C19 - C14	124.2(8)
C4 - C5 - C6	122(1)	O2 - C19 - C18	117.8(9)
C1 - C6 - C5	119.1(9)	C14 - C19 - C18	118.0(9)

Table 4 Hydrogen bond distances (H···acceptor) (Å) and angles (°)

Intra- molecular hydrogen bonds		
C13—H13....N3	2.425(3)	102.68(0)
Inter- molecular hydrogen bonds		
C10—H10....O1^{i}	2.550(0)	161.34(0)
C10—H10....O2^{i}	2.588(5)	133.90(0)

Symmetry code: (i) $-1/2+x$, $3/2-y$, $-1/2+z$.

ORTEP plot of the title complex is shown in Fig. 2. Table 2 shows final atomic coordinates while bond distances and bond angle are given in Table 3. The coordination of Cu(II) is from two oxygen atoms (O1, O2) and two nitrogen atoms (N1, N2); it is almost square planar. The Cu–N [1.928(7) – 1.933(7) Å] bond distances are longer than the Cu–O [1.880(6) – 1.890(5) Å]. The bond angles around Cu are in the range from 84.0(3) to 94.5(3)°.

We also observed that a weak intra- and inter-molecular hydrogen bonds as shown in Table 4.

References

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(Received December 18, 1996)
(Accepted February 20, 1997)