

Crystal and Molecular Structure of Hydroxynaphthoquinone Complex. I. The Structure of Bis (Pyridine) Bis (Lawson) Copper (II) Complex

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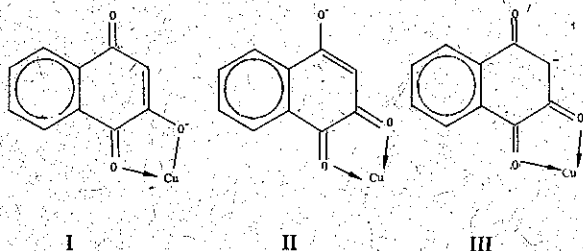
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ABSTRACT

The six-coordinate bis(pyridine)bis(lawson) copper(II) complex, $\text{Cu}(\text{py})_2(\text{Lw})_2$, has been synthesized and its structure determined by three dimensional X-ray diffraction data. The complex crystallized with one formula unit in the triclinic space group $C_1^1-P\bar{1}$ with $a=8.4847(12)$, $b=8.9940(4)$, $c=10.0190(4)$ Å, and $\alpha=73.224(4)$, $\beta=86.308(9)$, $\gamma=60.900(9)^\circ$. The final agreement indices on F, based on the least-squares refinement of 218 variables for 2290 observations $F \geq 3\sigma(F)$, are $R=0.041$, $R_w=0.046$. The bond pattern of the planar lawson anion has been found to exhibit some extent of delocalization. The coordinate geometry of the Cu(II) is found to be a tetragonal distorted octahedron with two pyridine nitrogen atoms and two hydroxy oxygen atoms as the square base and two carbonyl oxygen atoms as the apex. The bond distances of Cu-N, Cu-O (hydroxy), Cu-O (carbonyl) are 2.039(3), 1.945(2), and 2.454(2) Å, respectively.

Introduction

2-Hydroxy-1,4-naphthoquinone (Lawson, abbreviated as LwH) has found its application in qualitative and quantitative analyses of various metal ions including Cu(II) ion [1, 7, 8, 13]. Structural analyses of this $\text{Cu}(\text{py})_2(\text{Lw})_2$ complex was undertaken for two reasons: first, since several resonance forms of the anion of lawson can be drawn as follows:



we would like to establish the degree of delocalization (or the charge distribution) of the anion of lawson in the complex. Secondly, Cu(II) usually has a strong Jahn-Teller distortion. We are therefore deeply interested in the coordination geometry of the Cu(II) ion in this molecule. In other words, the questions of whether the two nitrogen atoms of pyridine or the two oxygen atoms of lawson occupy the apical positions, along with a study of their bond parameters, seem worthwhile to investigate.

Experimental Section

Preparation of Materials

All chemicals were reagent grade. Lawson were obtained from the Sigma Chemical Company.

$\text{Cu}(\text{Lw})_2$ [5] 0.45 g of lawson was dissolved in 50 ml of boiling 95% ethanol. To this was added 2.1 g of $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, dissolved in 50 ml warm, distilled water.

Table 1. Positional and Thermal Parameters for the Non-hydrogen Atoms of $\text{Cu}(\text{py})_2(\text{Lw})_2$

Atom	X ^a	Y	Z	U ₁₁ ^b	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Cu	0.0(0)	0.0(0)	0.0(0)	4.64(3)	4.26(3)	3.99(3)	-2.17(3)	1.22(2)	-1.08(2)
O1	0.2744(2)	-0.2798(2)	0.1123(2)	5.5(1)	5.5(1)	4.3(1)	-2.4(1)	1.7(1)	-1.1(1)
O2	-0.0327(2)	-0.0509(2)	0.1989(2)	5.2(1)	4.0(1)	4.2(1)	-1.8(1)	1.2(1)	-1.0(1)
O3	0.1170(3)	-0.4803(3)	0.6352(2)	9.9(2)	8.3(2)	4.6(1)	-2.7(1)	2.7(1)	-0.4(1)
N1	0.1195(3)	0.1419(3)	0.0221(2)	5.2(1)	5.0(1)	4.5(1)	-2.7(1)	1.1(1)	-1.2(1)
C1	0.2440(3)	-0.3272(3)	0.2337(3)	4.5(1)	4.3(1)	4.2(1)	-2.4(1)	1.0(1)	-1.4(1)
C2	0.0717(3)	-0.2038(3)	0.2860(2)	4.7(1)	4.4(1)	4.2(1)	-2.5(1)	1.2(1)	-1.6(1)
C3	0.0378(4)	-0.2616(4)	0.4196(3)	5.9(2)	5.2(2)	4.9(2)	-2.0(1)	2.0(1)	-1.5(1)
C4	0.1528(4)	-0.4327(4)	0.5148(3)	6.8(2)	6.1(2)	4.2(1)	-3.0(2)	1.5(1)	-1.1(1)
C5	0.3219(4)	-0.5574(4)	0.4643(3)	5.7(2)	4.8(2)	4.4(1)	-2.4(1)	0.4(1)	-1.2(1)
C6	0.4354(5)	-0.7271(4)	0.5512(3)	7.9(2)	5.6(2)	5.2(2)	-2.7(2)	0.5(2)	-0.5(1)
C7	0.5940(5)	-0.8395(4)	0.5055(4)	7.8(2)	4.8(2)	7.1(2)	-1.2(2)	-0.2(2)	-0.6(2)
C8	0.6418(5)	-0.7834(4)	0.3748(4)	6.2(2)	5.2(2)	8.1(2)	-1.2(2)	0.8(2)	-2.0(2)
C9	0.5304(4)	-0.6159(4)	0.2872(3)	5.3(2)	5.2(2)	5.7(2)	-2.1(1)	1.1(1)	-1.7(1)
C10	0.3689(4)	-0.5027(3)	0.3307(3)	4.8(2)	4.4(1)	4.6(1)	-2.4(1)	0.6(1)	-1.5(1)
C11	0.0813(5)	0.2233(4)	-0.1228(3)	7.7(2)	6.6(2)	5.8(2)	-4.3(2)	2.5(2)	-2.5(2)
C12	0.1621(6)	0.3167(5)	0.1406(4)	11.4(3)	9.8(3)	7.1(2)	-7.5(3)	3.0(2)	-4.4(2)
C13	0.2883(6)	0.3283(6)	0.0532(4)	11.5(3)	11.0(3)	6.4(2)	-8.5(3)	1.3(2)	-2.9(2)
C14	0.3314(5)	0.2453(5)	-0.0492(4)	8.3(2)	11.3(3)	6.8(2)	-7.2(2)	2.4(2)	-3.2(2)
C15	0.2448(4)	0.1535(4)	-0.0623(3)	6.6(2)	8.3(2)	5.8(2)	-4.7(2)	2.1(2)	-2.8(2)

^aEstimated standard deviations in the least significant figures are given in parentheses.

^bThe form of the anisotropic thermal ellipsoid is $\exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}hla^*c^* + 2U_{23}klb^*c^*) \times 10^{-2}]$.

The solution changed color from the pale yellow of the ligand to the red of the complex. The complex precipitated when the solution cooled. The precipitate was filtered, washed several times with distilled water and 95% ethanol and yielded 0.6 g of $\text{Cu}(\text{Lw})_2$. The I.R. spectrum is identical to that given in ref. 5. Attempts to grow single crystals of this compound were unsuccessful.

$\text{Cu}(\text{py})_2(\text{Lw})_2$ 0.5 g of $\text{Cu}(\text{Lw})_2$ was dissolved in 20 ml of pyridine. To this was slowly added 40 ml of ether. A red precipitate was obtained. It was then filtered and washed with ether. Anal. Calcd for $\text{Cu}(\text{py})_2(\text{Lw})_2$: C, 63.43%; H, 3.55%; N, 4.93%. Found: C, 63.32%; H, 3.25%; N, 5.21%. Crystals of $\text{Cu}(\text{py})_2(\text{Lw})_2$, suitable for X-ray study, were grown by slow diffusion of ether into a saturated pyridine solution of $\text{Cu}(\text{Lw})_2$ for one to two days.

Crystallographic data

The crystals are prone to decompose outside of the pyridine solution, presumably with loss of pyridine coordination. This problem was solved by covering the crystal completely with epoxy resin.

Preliminary precession photographs of the crystals displayed triclinic symmetry with the P1 or P1̄ space group. The cell parameters obtained by centering 25 reflections with θ range from 18° to 55° are $a=8.4847(12)$, $b=8.9940(4)$, $c=10.0190(4)$ Å, and $\alpha=73.224(4)$, $\beta=86.308(9)$, $\gamma=60.900(9)^\circ$. The calculated density, based on one $\text{Cu}(\text{py})_2(\text{Lw})_2$ molecule per unit cell is 1.481 g/cm³ and agrees well with an observed value of 1.48(2) g/cm³, as measured by floatation in CHCl_3 and CCl_4 solution.

2409 unique intensity data with 2θ range from 4° to 140° were obtained on a 4-circle diffractometer (CAD4) with θ - 2θ scan technique. Using Cu K α radiation 2290 reflections were found to have $F \geq 3\sigma(F)$ and used in the later refinement. The scan parameters are $\Delta\theta = 1.0 + 0.14(\tan\theta)$ with scan speed 20/3 deg/min. The backgrounds were taken with quarter of total scanning time at each end of the scan limit.

Solution and Refinement of Structure

The Cu atom was put at the origin by assuming P1̄ space group and one molecule per unit cell. Subsequent Fourier synthesis led to the location of all non-hydrogen atoms. The structure was refined by full-matrix, least-

Table 2. Positional and Thermal Parameters for the Hydrogen Atoms of $\text{Cu}(\text{py})_2(\text{Lw})_2$

Atom	X ^a	Y	Z	U ^b
H1	-0.073(4)	-0.193(4)	0.452(3)	3.7(9)
H2	0.394(4)	-0.766(4)	0.632(3)	4.5(10)
H3	0.670(4)	-0.964(4)	0.567(3)	4.4(9)
H4	0.751(5)	-0.848(4)	0.338(3)	5.3(10)
H5	0.553(4)	-0.577(4)	0.206(3)	2.9(9)
H6	-0.016(4)	0.215(4)	0.179(3)	4.9(9)
H7	0.127(5)	0.368(5)	0.209(4)	6.0(11)
H8	0.346(5)	0.387(5)	0.064(4)	7.7(14)
H9	0.417(5)	0.243(5)	-0.108(4)	5.4(11)
H10	0.283(4)	0.077(4)	-0.127(3)	5.2(10)

^aEstimated standard deviations in the least significant figures are given in parentheses.

^bThe form of isotropic thermal ellipsoid is $\exp\{-8\pi^2U\sin^2\theta/\lambda^2\} \times 10^{-2}$.

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squares technique. The usual procedures, computer program, atomic scattering factors, and anomalous terms were employed [2]. In the final refinement, all the non-hydrogen atoms were refined anisotropically and the hydrogen atoms refined isotropically. The final agreement indices on F for the 2290 reflections and 218 variables are $R=0.041$, $R_w=0.046$. The final difference Fourier is featureless with maximum peak of $0.2 \text{ e}/\text{\AA}^3$. The final positional and thermal parameters for the non-hydrogen atoms are shown in Table 1. The parameters for hydrogen atoms are given in Table 2.

Description of the Structure and Discussion

The crystal structure consists of discrete molecules of $\text{Cu}(\text{py})_2(\text{Lw})_2$. Which are shown in Fig. 1, and a view of the $\text{Cu}(\text{py})_2(\text{Lw})_2$ molecule with atom numbering scheme used is shown in Fig. 2. In Table 3 the bond distances and angles in the $\text{Cu}(\text{py})_2(\text{Lw})_2$ molecule are presented. The six-coordinated Cu(II) complex is formed by coordination of two bidentate ligands of lawson anion and two pyridine molecules. The Cu(II) ion is located at center of symmetry. The two anions of lawson and the two pyridine are related by the center of symmetry.

In this complex, anion of lawson is planar. Table 4 gives their equations of least-square plane and the deviations from planarity for each atoms. The benzene ring formed by C5-C6-C7-C8-C9-C10 six atoms still remains aromatic on coordination. The bonds C1-C2 (1.517(3) Å), C4-C5 (1.497(4) Å), and C10-C1 (1.477(3) Å) are not affected by coordination. In other words, they exist as single bonds. The most interesting features are the bond lengths of C2-C3, C3-C4, O1-C1, O2-C2, and O3-C4, because they are closely related with the so-called bond delocalization or charge distribution. The bond C2-C3 (1.356(4) Å) is slightly longer than the C=C double bond in benzoquinone [14] and quinhydrone [12] (1.322 Å and 1.33 Å respectively), the bond C3-C4 (1.429(3) Å), however, is shorter than the C-C single bond in benzoquinone [14] and quinhydrone [12] (1.477 and 1.487 Å). Similarly, the bond O2-C2 (1.288(2) Å) is much shorter than the C-O single bond in quinhydrone [12], catechol

Table 3. Intramolecular Bond Distances and Angles in $\text{Cu}(\text{py})_2(\text{Lw})_2$

Atoms	Distance, Å	Atoms	Distance, Å
Cu-O1	2.454(2)	C8-C9	1.375(4)
Cu-O2	1.945(2)	C9-C10	1.388(4)
Cu-N1	2.039(3)	C11-C12	1.367(8)
O1-C1	1.222(3)	C12-C13	1.364(7)
O2-C2	1.288(2)	C13-C14	1.367(7)
O3-C4	1.230(4)	C14-C15	1.380(8)
N1-C11	1.346(5)	H1-C3	0.94(3)
N1-C15	1.340(4)	H2-C6	0.90(3)
C1-C2	1.517(3)	H3-C7	1.00(3)
C1-C10	1.477(3)	H4-C8	0.94(3)
C2-C3	1.356(4)	H5-C9	0.84(3)
C3-C4	1.429(3)	H6-C11	0.99(4)
C4-C5	1.497(4)	H7-C12	0.89(4)
C5-C6	1.388(4)	H8-C13	0.91(6)
C5-C10	1.391(4)	H9-C14	0.90(4)
C6-C7	1.381(5)	H10-C15	1.01(4)
C7-C8	1.372(5)		
Atoms	Angle, deg	Atoms	Angle, deg
O1-Cu-O2	74.80(6)	H3-C7-C8	121(2)
O1-Cu-N1	90.45(8)	C6-C7-C8	120.3(3)
O2-Cu-N1	89.90(10)	H4-C8-C7	126(2)
Cu-O1-O2	105.8(1)	H4-C8-C9	114(2)
Cu-O2-C2	121.4(2)	C7-C8-C9	120.2(3)
Cu-N1-C11	122.3(2)	H5-C9-C8	123(2)
Cu-N1-C15	120.6(2)	H5-C9-C10	117(2)
O1-C1-C2	119.3(2)	C1-C10-C5	120.0(2)
O1-C1-C10	121.9(2)	C1-C10-C9	120.1(2)
C2-C1-C10	118.8(2)	C5-C10-C9	119.9(2)
O2-C2-C3	124.7(2)	H6-C11-C12	123(2)
O2-C2-C1	117.0(2)	H6-C11-N1	114(2)
C1-C2-C3	118.3(2)	N1-C11-C12	123.2(4)
H1-C3-C2	120(2)	H7-C12-C11	117(3)
H1-C3-C4	115(2)	H7-C12-C13	124(3)
C2-C3-C4	124.3(2)	C11-C12-C13	119.0(4)
O3-C4-C3	122.3(3)	H8-C13-C12	121(2)
O3-C4-C5	119.5(2)	H8-C13-C14	120(2)
C3-C4-C5	118.2(2)	C12-C13-C14	119.2(6)
C4-C5-C6	120.5(2)	H9-C14-C13	124(3)
C4-C5-C10	120.2(2)	H9-C14-C15	117(3)
C6-C5-C10	119.3(2)	C13-C14-C15	119.2(4)
H2-C6-C5	118(2)	H10-C15-N1	115(2)
H2-C6-C7	122(2)	H10-C15-C14	122(2)
C5-C6-C7	120.2(3)	C14-C15-N1	122.4(4)
H3-C7-C6	119(2)		

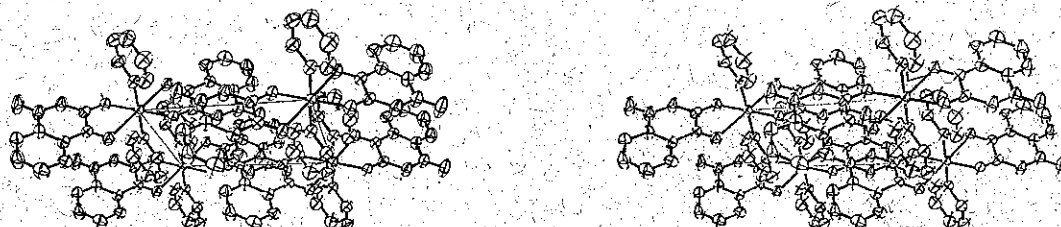
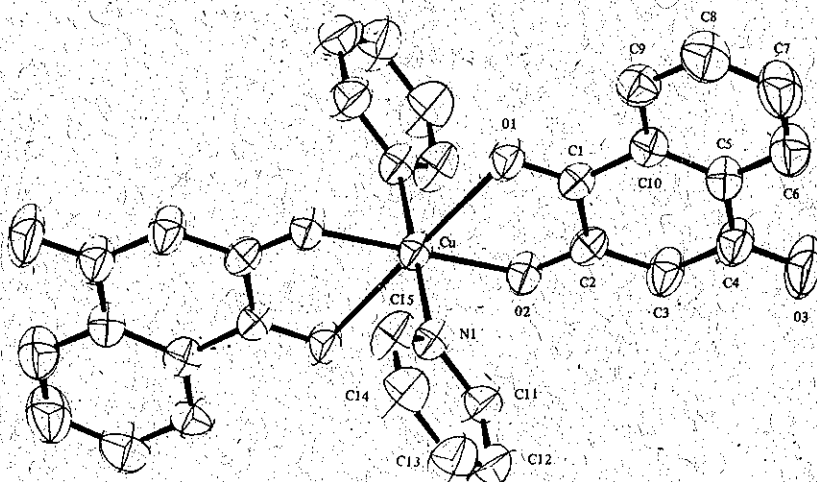
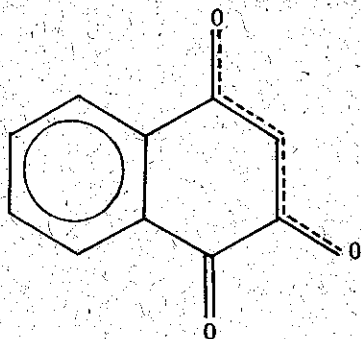


Fig. 1. Stereo Views of Crystal Structure of $\text{Cu}(\text{py})_2(\text{Lw})_2$.

Fig. 2. The ORTEP plot of the molecule $\text{Cu}(\text{py})_2(\text{Lw})_2$ and the numbering scheme.

[6], hydroquinone [10], and tetrahydroxy-p-benzoquinone [9] (1.41 Å, 1.372 Å, 1.393 Å, and 1.344 Å, respectively). The bonds O3-C4 (1.230(4) Å) and O1-C1 (1.222(3) Å) are almost equal to the C=O double bond in benzoquinone [14] quinhydrone [12], and tetrahydroxy-p-benzoquinone [9] (1.222, 1.23, and 1.229 Å, respectively). All these results indicate the existence of some degree of delocalization along the five atoms of O3-C4-C3-C2-O2:



The bond parameters in pyridine molecule are normal. The equation of the least-squares plane and the deviations from the plane are given in Table 4. The pyridine ring is not exactly perpendicular to the plane of the lawsonone. The dihedral angle between these two planes is 80° .

The inner coordination sphere of the complex, with selected bond parameters, is shown in Fig. 3. The environment of the central copper atom is an axially distorted octahedron with two pyridine nitrogen atoms and two hydroxy oxygen atoms as the square base and two carbonyl oxygen atoms as the apex. The Cu-N(pyridine) distance 2.039(3) Å may be compared with Cu-N(ammonia) distance 2.05(1) Å found in $\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})\text{SO}_4$ [11]; Cu-N(pyridine) 2.02(1) Å in diaquabis(N-acetyl-tryptophanato) bis(pyridine) Cu(II) [4].

The Cu-O(hydroxy) distance 1.945(2) Å may also be compared with Cu-O(water) distance of 1.94-1.99 Å found in $\text{Cu}(\text{H}_2\text{O})_4\text{SO}_4(\text{H}_2\text{O})$ [3]; Cu-O(carboxylate) distance 1.95(1) Å in diaquabis(N-acetyl-tryptophanato) bis(pyridine) Cu(II) [4]. The long axial Cu-O(carbonyl) bond distance 2.454(2) Å may be compared with Cu-O(water) distance of 2.59 Å in $\text{Cu}(\text{NH}_3)_4(\text{H}_2\text{O})\text{SO}_4$ [11]; Cu-O(water) distance of 2.61(1) Å in diaquabis(N-acetyl-tryptophanato) bis(pyridine) Cu(II) [4].

The results of single crystal analysis of $\text{Cu}(\text{py})_2(\text{Lw})_2$

Table 4. Deviations from the Least-Square Planes

Atom	Plane 1	Plane 2
Cu ^a	-0.42 Å	0.03 Å
O1	-0.06(4)	
O2	-0.01(4)	
O3	0.02(4)	
C1	-0.00(4)	
C2	0.00(4)	
C3	0.02(4)	
C4	0.01(4)	
C5	-0.02(4)	
C6	-0.06(4)	
C7	-0.05(4)	
C8	-0.03(4)	
C9	0.07(4)	
C10	0.04(4)	
N1		-0.004(3)
C11		0.004(3)
C12		0.001(3)
C13		-0.004(3)
C14		0.003(3)
C15		-0.001(3)

Coefficients of the Plane Equation $PX+QY+RZ=S$ ^b

Plane	P	Q	R	S
1	6.826	7.440	5.069	0.419
2	3.246	-3.647	4.256	-0.031

^a Cu atom was not included in the calculation of the plane.

^b The plane is in crystal coordinates.

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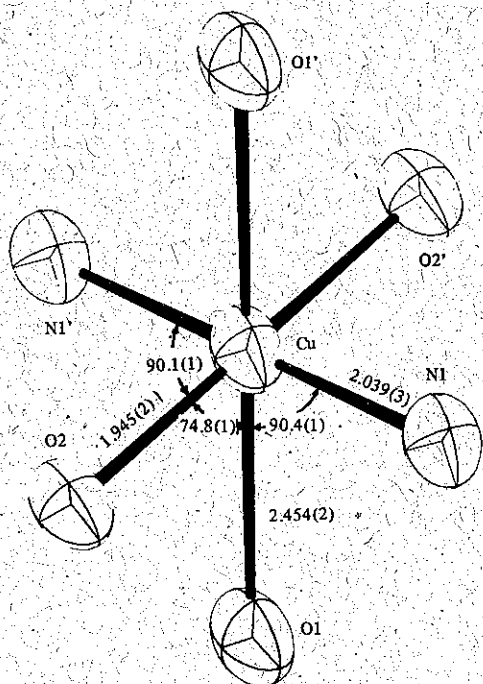


Fig. 3. The Inner Coordination Sphere of Cu(II) in $\text{Cu}(\text{py})_2(\text{Lw})_2$ complex lead us to believe that the lawsonone anions do have some degree of delocalization along O3-C4-C3-C2-O2 atoms when they are coordinated to the central Cu(II) ion and that the six-coordinated Cu(II) ion (d^9 configuration) does show strong Jahn-Teller distortion.

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羥基萘奎酮(hydroxynaphthoquinone)之結晶及分子構造(第一報) 雙吡啶雙嘍啶銅錯合物(bis(pyridine)bis(lawsone)Cu(II))之構造

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摘 要

新合成之六個配位數的雙吡啶雙嘍啶銅(bis(pyridine)bis(lawsone)Cu(II))錯合物之結晶構造,已由X光之繞射數據解析而得。這錯合物之結晶單元為三斜晶系,空間群為Pi,單元參數為 $a=8.4847(12)$, $b=8.9940(4)$, $c=10.0190(4)$ Å, $\alpha=73.224(4)$, $\beta=86.308(9)$, $\gamma=60.900(9)^\circ$ 。根據218個變數,2290個繞射數據之最小平方精算所得誤差指數 $R=0.041$ 及 $R_w=0.046$ 。整個構造而言,平面之嘍啶(lawsone)陰離子其鍵型有某種程度之非常局部件,銅離子之配位幾何型狀為四方扭曲八面體,其中兩個吡啶氮原子及兩個羥基氧原子形成四方底座,而兩個羰基氧原子在軸上,它們的鍵長分別為:Cu-N是 $2.039(3)$ Å, Cu-O(羥基)是 $1.945(2)$ Å, Cu-O(羰基)是 $2.454(2)$ Å。