

Dong-Yan Xu,<sup>a,b</sup> Ying Liu,<sup>b</sup>  
Ming-Li Liu,<sup>b</sup> Jun-Fa Wei<sup>a</sup> and  
Jian-Min Dou<sup>b\*</sup><sup>a</sup>School of Chemistry and Materials Science,  
Shanxi Normal University, Xian 710062,  
People's Republic of China, and <sup>b</sup>School of  
Chemistry and Chemical Engineering,  
Liaocheng University, Liaocheng 252059,  
People's Republic of China

Correspondence e-mail: jmdou@lctu.edu.cn

## Key indicators

Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 $R$  factor = 0.045  
 $wR$  factor = 0.117  
Data-to-parameter ratio = 12.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**[2-Oxido-1-naphthaldehyde (2-hydroxy-  
benzoyl)hydrazonato]pyridinecopper(II)**

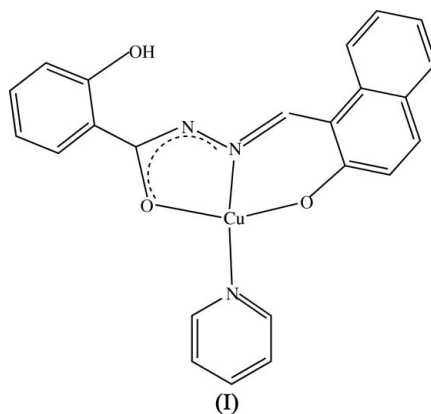
The approximately planar complex molecule,  $[\text{Cu}(\text{C}_{18}\text{H}_{12}\text{N}_2\text{O}_3)(\text{C}_5\text{H}_5\text{N})]$ , contains one  $L^{2-}$  ligand ( $L^{2-}$  is the dianion of 2-hydroxy-1-naphthaldehyde 2-hydroxybenzoylhydrazone), one Cu atom and one pyridine molecule. The Cu centre shows square-planar  $\text{N}_2\text{O}_2\text{Cu}$  coordination. The tridentate dianion has an intramolecular  $\text{N}\cdots\text{H}-\text{O}$  hydrogen bond. Each pair of adjacent molecules is linked together by  $\pi-\pi$  stacking and  $\text{Cu}\cdots\text{N}$  interactions, which lead to the existence of a dimer. Owing to  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds, these dimers are further assembled into a two-dimensional framework.

Received 18 February 2006

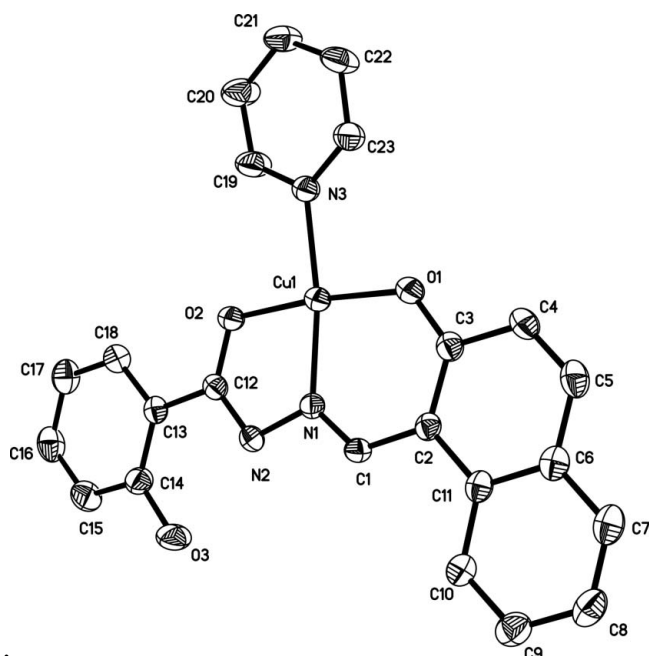
Accepted 23 February 2006

## Comment

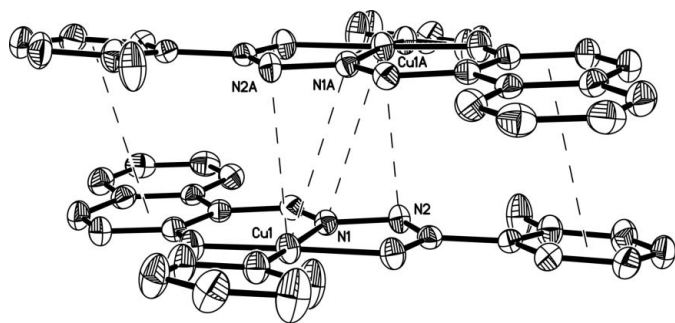
Interest in the chemistry of aroylhydrazones arises from their ability to bind to metal ions (Singh *et al.*, 1982; Salem, 1998) as well as their biological activity (Singh *et al.*, 1982; Carcelli *et al.*, 1995). In fact, with some hydrazones, their metal complexes are endowed with significantly improved biological and pharmaceutical activity (Ainscough *et al.*, 1998; Anford *et al.*, 1998). In particular, the copper complex of salicylaldehyde benzoylhydrazone possesses exceptional antibacterial activity (Ainscough *et al.*, 1998). The coordination chemistry of copper hydrazone complexes, such as  $[\text{Cu}(\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}_3)(\text{C}_5\text{H}_5\text{N})]$  (Chen *et al.*, 2004),  $[\text{Cu}(\text{H}_2\text{sb})(\text{CCl}_3\text{CO}_2)_2]_2$  (Ainscough *et al.*, 1998), and  $[\text{Cu}_4(\text{POAPZ-H})_4(\text{H}_2\text{O})_2](\text{NO}_3)_4\cdot 4\text{H}_2\text{O}$  and  $[\text{Cu}_4(\text{POAP-H})_4](\text{ClO}_4)_4$  (POAPZ-H is *N*-imidopyrazine picolinic hydrazide and POAP-H is *N*-imidopicoline picolinic hydrazide; Matthews *et al.*, 1999), have been reported. The present study describes the title compound, (I) (Fig. 1).



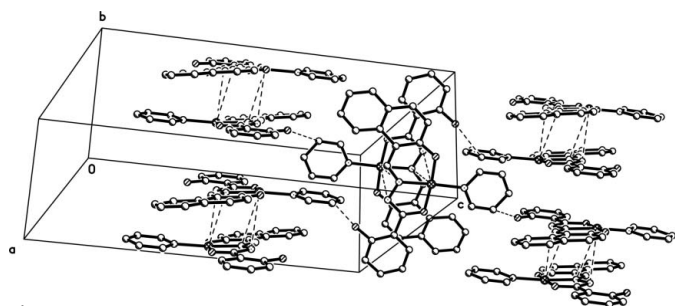
The complex, (I), contains one  $L^{2-}$  ligand, one Cu atom and one pyridine molecule. The geometry around the Cu centre can be described as a square plane composed of the  $\text{N}_2\text{O}_2$  set of atoms; the two O atoms and one N atom are supplied by the tridentate  $L^{2-}$ , while the other N atom comes


**Figure 1**

The molecular structure of the title complex. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity.


**Figure 2**

The dimer structure formed by Cu...N and  $\pi$ - $\pi$  interactions (dashed lines). [Symmetry code: (A)  $1 - x, 1 - y, 2 - z$ ]. H atoms have been omitted.


**Figure 3**

The crystal packing of the title complex. Dashed lines indicate hydrogen bonds.

from the pyridine molecule. The free hydroxy group forms an intramolecular hydrogen bond. The two chelate rings are nearly coplanar.

Inversion-related pairs of molecules are linked together by weak Cu...N interactions, with Cu1...N1<sup>i</sup> and Cu1...N2<sup>i</sup>

separations of more than 3.2 Å [symmetry code: (i)  $1 - x, 1 - y, -z$ ]. As with [Ni(C<sub>18</sub>H<sub>12</sub>N<sub>2</sub>O<sub>3</sub>)(C<sub>5</sub>H<sub>5</sub>N)] (Liu *et al.*, 2005), there are  $\pi$ - $\pi$  interactions between each pair of naphthalene and phenyl ring planes, giving rise to a weakly held dimer (Fig. 2).

The packing of (I) (Fig. 3) shows that atom C20 interacts with atom O3<sup>i</sup> at a distance of 3.347 (5) Å [symmetry code: (i)  $x, \frac{1}{2} - y, z + \frac{1}{2}$ ], and this weak interaction leads to the formation of a layer motif in the *bc* plane.

## Experimental

The ligand *L* (0.25 mmol, 0.077 g), KOH (0.5 mmol, 0.028 g), Cu(ClO<sub>4</sub>)<sub>2</sub> (0.25 mmol, 0.086 g), dimethylformamide (8 ml) and methanol (8 ml) were mixed. After stirring the solution for about 4 h, the green precipitate which formed was dissolved in pyridine (10 ml). A week later, dark-green crystals of (I) were isolated from the solution [m.p. >573 K (decomposition)]. Spectroscopic analysis: FT-IR (KBr pellets,  $\nu$ , cm<sup>-1</sup>): 3443 (s), 3047 (w), 1615 (vs), 1602 (s), 1527 (s), 1452 (s), 1484 (s), 1391 (s), 1334 (s), 1256 (s), 1302 (m), 1239 (w), 1138 (m), 1017 (s), 971 (m), 855 (w), 757 (vs), 696 (s), 676 (m), 526 (m), 452 (m).

### Crystal data

[Cu(C<sub>18</sub>H<sub>12</sub>N<sub>2</sub>O<sub>3</sub>)(C<sub>5</sub>H<sub>5</sub>N)]  
*M<sub>r</sub>* = 446.94  
 Monoclinic, *P*<sub>2</sub><sub>1</sub>/*c*  
*a* = 11.745 (2) Å  
*b* = 8.1666 (17) Å  
*c* = 20.380 (4) Å  
 $\beta$  = 105.397 (3)°  
*V* = 1884.5 (7) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.575 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 2185 reflections  
 $\theta$  = 2.4–22.8°  
 $\mu$  = 1.19 mm<sup>-1</sup>  
*T* = 298 (2) K  
 Block, dark green  
 0.28 × 0.21 × 0.12 mm

### Data collection

Siemens SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.732, *T<sub>max</sub>* = 0.870  
 9587 measured reflections

3369 independent reflections  
 2557 reflections with  $I > 2\sigma(I)$   
*R<sub>int</sub>* = 0.038  
 $\theta_{\text{max}}$  = 25.2°  
*h* = -10 → 14  
*k* = -9 → 9  
*l* = -23 → 24

### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.045  
*wR*(*F*<sup>2</sup>) = 0.117  
*S* = 1.02  
 3369 reflections  
 271 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0671P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.42 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.22 \text{ e } \text{Å}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Cu1—O1	1.880 (2)	N1—N2	1.395 (3)
Cu1—N1	1.904 (3)	N2—C12	1.319 (4)
Cu1—O2	1.922 (2)	O1—C3	1.302 (4)
Cu1—N3	1.997 (3)	O2—C12	1.288 (3)
N1—C1	1.284 (4)	O3—C14	1.353 (4)
O1—Cu1—N1	92.75 (10)	O1—Cu1—N3	93.94 (10)
O1—Cu1—O2	173.84 (9)	N1—Cu1—N3	171.13 (11)
N1—Cu1—O2	81.66 (10)	O2—Cu1—N3	91.89 (10)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C20-H20\cdots O3^{ii}$	0.93	2.81	3.347 (5)	118

Symmetry code: (ii)  $x, -y + \frac{1}{2}, z + \frac{1}{2}$ .

All H atoms were positioned geometrically and refined as riding on their parent atoms;  $C-H = 0.93 \text{ \AA}$  and  $U_{iso}(H) = 1.2U_{eq}(C)$ , and  $O-H = 0.82 \text{ \AA}$  and  $U_{iso}(H) = 1.5U_{eq}(O)$ .

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the support of the Natural Science Foundation of Shandong Province, China (grant No. Y2003B01).

**References**

- Anford, J. D., Vittal, J. J. & Wang, Y. M. (1998). *Inorg. Chem.* **37**, 1226–1231.
- Ainscough, E. W., Brodie, A. M., Dobbs, A. J., Ranford, J. D. & Waters, J. M. (1998). *Inorg. Chim. Acta*, **267**, 27–38.
- Carcelli, M., Mazza, P., Pelizzi, C., Pelizzi, G. & Zani, F. (1995). *J. Inorg. Biochem.* **57**, 43–62.
- Chen, X. H. & Liu, S. X. (2004). *Chin. J. Inorg. Chem.* **20**, 668–670.
- Matthews, C. J., Avery, K., Xu, Z. Q., Thompson, L. K., Zhao, L., Miller, D. O., Biradha, K., Poirier, K., Zaworotko, M. J., Wilson, C., Goeta, A. E. & Howard, J. A. K. (1999). *Inorg. Chem.* **38**, 5266–5276.
- Liu, M.-L., Dou, J.-M., Wang, D.-Q. & Li, D.-C. (2005). *Acta Cryst.* **E61**, m1366–m1367.
- Salem, A. A. (1998). *Microchem. J.* **60**, 51–66.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997a). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997b). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
- Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Singh, R. B., Jain, P. & Singh, R. P. (1982). *Talanta*, **29**, 77–84.