

Hapipah M. Ali,<sup>a</sup> Mohd Idris  
Najwa,<sup>a</sup> Ming-Jin Xie<sup>b</sup> and  
Seik Weng Ng<sup>a\*</sup><sup>a</sup>Department of Chemistry, University of Malaya,  
50603 Kuala Lumpur, Malaysia, and <sup>b</sup>School  
Chemistry, Yunnan University, Kunming  
650092, People's Republic of China

Correspondence e-mail: seikweng@um.edu.my

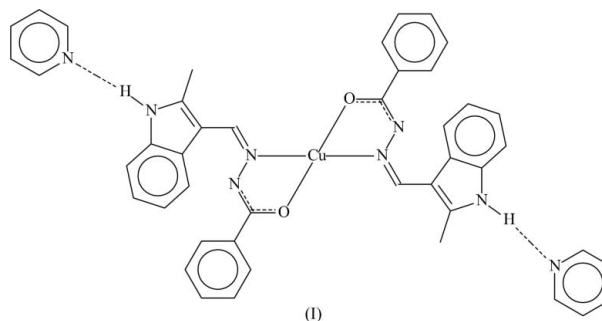
## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.036  
 $wR$  factor = 0.105  
Data-to-parameter ratio = 15.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis(2-methyl-1*H*-indole-3-carbaldehyde  
benzoylhydrazonato- $\kappa^2N,O$ )copper(II)  
pyridine disolvateThe Cu atom in the title compound,  $[\text{Cu}(\text{C}_{17}\text{H}_{14}\text{N}_3\text{O})_2] \cdot 2\text{C}_5\text{H}_5\text{N}$ , is chelated by the deprotonated Schiff base in a square-planar geometry; the amine group of the Schiff base forms a hydrogen bond with a pyridine solvent molecule. The Cu atom lies on a center of inversion.

Received 12 September 2006

Accepted 13 September 2006

## Comment

The copper derivative of the 5-bromo-1*H*-indole-3-carbaldehyde 2-nitrobenzoylhydrazonate Schiff base, when purified from *N,N*-dimethylformamide, has two deprotonated ligands in a square-planar geometry around the metal atom. The solvent molecules are positioned above and below the square plane at a long distance [3.014 (4) Å] (Ali *et al.*, 2006). The title compound when purified from pyridine crystallizes as a pyridine disolvate, (I) (Fig. 1); however, the solvent molecules do not interact directly with the metal atom, which is in its commonly observed square-planar coordination. Instead, the solvent molecule forms a hydrogen bond with the amine group (Table 1).

## Experimental

The Schiff base was synthesized in ethanol (100 ml) by condensing 2-methylindole-3-carboxaldehyde (0.6 g, 3.8 mmol) with benzhydrazide (0.51 g, 0.38 mmol). The mixture was refluxed for 2 h. The solvent was then removed to give the organic ligand. 2-Methyl-1*H*-indole-3-carbaldehyde benzoylhydrazine (0.24 g, 0.9 mmol) and copper(II) acetate dihydrate (0.09 g, 0.45 mmol) were heated in ethanol (100 ml) for 5 h. The solvent was removed and the solid material recrystallized from pyridine.

## Crystal data

 $[\text{Cu}(\text{C}_{17}\text{H}_{14}\text{N}_3\text{O})_2] \cdot 2\text{C}_5\text{H}_5\text{N}$  $M_r = 774.36$ Monoclinic,  $C2/c$  $a = 22.552$  (2) Å $b = 9.076$  (1) Å $c = 19.107$  (2) Å $\beta = 100.503$  (1)° $V = 3845.5$  (5) Å<sup>3</sup> $Z = 4$  $D_x = 1.338$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation $\mu = 0.62$  mm<sup>-1</sup> $T = 293$  (2) K

Fragment, brown

 $0.36 \times 0.23 \times 0.17$  mm

## Data collection

Bruker APEX-II area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.783$ ,  $T_{\max} = 0.902$

16507 measured reflections  
 3943 independent reflections  
 3103 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.028$   
 $\theta_{\text{max}} = 26.4^\circ$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.105$   
 $S = 1.02$   
 3943 reflections  
 255 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 1.8992P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.21 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.25 \text{ e } \text{Å}^{-3}$

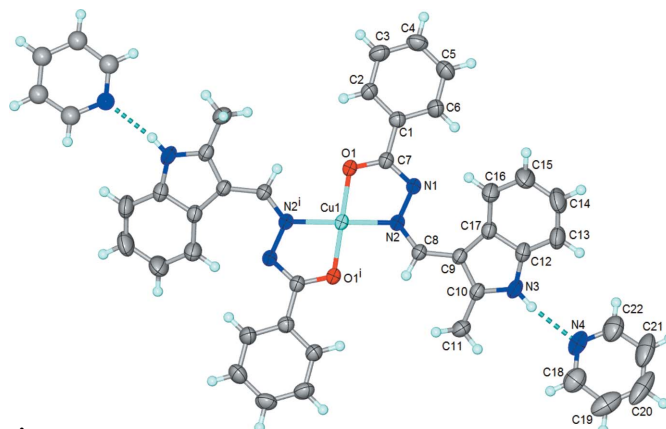
**Table 1**

Hydrogen-bond geometry ( $\text{Å}$ ,  $^\circ$ ).

| $D-H\cdots A$     | $D-H$    | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------|----------|-------------|-------------|---------------|
| $N3-H3n\cdots N4$ | 0.85 (1) | 2.07 (1)    | 2.910 (3)   | 169 (3)       |

The carbon-bound H atoms were placed at calculated positions ( $C-H = 0.93-0.98 \text{ Å}$ ) and included in the refinement in the riding-model approximation, with  $U_{\text{iso}}(\text{H})$  values set at 1.2 or 1.5 times  $U_{\text{eq}}(\text{C})$ . The methyl group was rotated to fit the electron density. The amine H atom was located in a difference Fourier map and refined with a distance restraint [ $N-H = 0.85 (1) \text{ Å}$ ]; its displacement parameter was refined.

Data collection: *APEXII* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-*



**Figure 1**

The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level and H atoms as spheres of arbitrary radii. The dashed lines represent the N—H $\cdots$ N hydrogen bonds. [Symmetry code: (i)  $\frac{1}{2} - x, \frac{3}{2} - y, 1 - z$ .]

*SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

The authors thank the Scientific Advancement Grant Allocation (No. 66-02-03-0046/Oracle 815-0046) and the University of Malaya for supporting this study.

## References

- Ali, M. H., Abdul Halim, S. N. & Ng, S. W. (2006). *Acta Cryst.* **E62**, m724–m725.  
 Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.  
 Bruker (2004). *APEXII* (Version 7.23A) and *SAINT* (Version 7.23A). Bruker AXS Inc., Madison, Wisconsin, USA.  
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.