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# *catena*-Poly[copper(I)-$\mu$-2-(2-pyridyl)-1*H*-benzimidazolato-$\kappa^2N^1:N^3$]

**Ming-Hua Zeng,[a] Xing-Can Shen[a] and Seik Weng Ng[b]***

[a]Department of Chemistry, Guangxi Normal University, Guilin 541000, Guangxi, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

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

**Key indicators**

Single-crystal X-ray study
*T* = 295 K
Mean $\sigma$() = 0.000 Å
Disorder in main residue
*R* factor = 0.041
*wR* factor = 0.125
Data-to-parameter ratio = 9.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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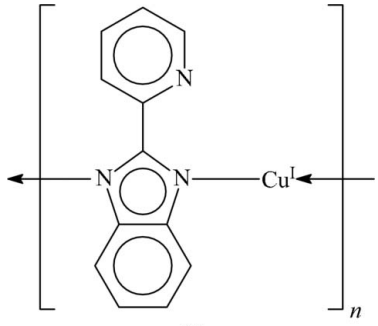
The chain structure of the title compound, $[Cu(C_{12}H_8N_3)]_n$, consists of alternating 2-(2-pyridyl)-1*H*-benzimidazolate anions and copper(I) cations. The chain, which has the $Cu^I$ atom in a linear coordination geometry, runs along the *a* axis of the monoclinic unit cell.

## Comment

2-(2-Pyridyl)-1*H*-benzimidazole, a luminescent compound whose crystal structure has been reported (Yue *et al.*, 2003), forms adducts with a number of metal salts. With some, the ligand binds through the imidazolyl Lewis-basic site, whereas in others, the ligand chelates through the imidazolyl and pyridyl sites (Battaglia *et al.*, 1976; Casas *et al.*, 2005; Choquesillo-Lazarte *et al.*, 2002; Dave & Czernuszewicz, 1996; Kabanos *et al.*, 1992; Maekawa *et al.*, 1994; Mock *et al.*, 2001; Müller-Buschbaum, 2002; Müller-Buschbaum & Quitmann, 2003, 2004; Munakata *et al.*, 1997; Peng & Chen, 1990; Sokolov *et al.*, 2005; Tangoulis *et al.*, 1996; Yue *et al.*, 2006). The ligand exists in the neutral form in these examples. Interestingly, under hydrothermal conditions, the ligand reacts with the copper(II) cation, which undergoes reduction to the copper(I) cation, which then binds to the deprotonated ligand to furnish a linear chain structure for (I) (Fig. 1).




(I)

The metal atom is two-coordinate in a linear geometry. The pyridyl rings are positioned to be within van der Waals interaction with it, but their basic nitrogen sites do not interact to form bonds. The Cu—N bonds are relatively short, but compare well with those found in $\mu_2$-benzimidazolato complexes of copper(I) (Kolks & Lippard, 1984; Plass *et al.*, 2002).

## Experimental

The 2-(3-pyridyl)-1*H*-benzimidazole ligand was synthesized by using the method developed for 2-(4-pyridyl)-1*H*-benzimidazole trihydrate

(Huang *et al.*, 2004). Picolinic acid (1.25 g, 10 mmol) and 1,2-diaminobenzene (1.08 g, 10 mmol) were added to polyphosphoric acid (14 g). The mixture was heated under nitrogen at 433 K for 8 h to give a viscous syrup. The syrup was poured into 500 ml water. The tan solid that separated was collected and suspended in 500 ml 0.5 *M* sodium carbonate. The product was collected and air dried. The copper complex was synthesized hydrothermally from equimolar quantitites of the amine (0.195 g, 1 mmol) and copper(II) nitrate trihydrate (0.242 g, 1 mmol); the reactants were placed in 25% ammonium hydroxide (5 ml). The mixture was placed in a 15 ml Teflon-lined stainless steel bomb. The bomb was heated at 423 K for 72 h. The bomb was cooled to room temperature at a rate of 10 K $min^{-1}$. Yellow rod-shaped crystals were isolated by hand (yield *ca* 20%, based on Cu).

### *Crystal data*

$[Cu(C_{12}H_8N_3)]$
$M_r$ = 257.75
Monoclinic, $P2_1/c$
$a$ = 5.858 (1) Å
$b$ = 22.090 (3) Å
$c$ = 8.212 (1) Å
$\beta$ = 109.255 (2)°
$V$ = 1003.2 (2) $Å^3$
$Z$ = 4
$D_x$ = 1.707 Mg $m^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 2.15 $mm^{-1}$
$T$ = 295 (2) K
Rod, yellow
0.21 × 0.12 × 0.10 mm

### *Data collection*

Bruker SMART 1000 area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.661, $T_{max}$ = 0.814
6798 measured reflections
2181 independent reflections
1913 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.018
$\theta_{max}$ = 27.0°

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.125
$S$ = 1.04
2181 reflections
232 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.084P)^2 + 0.692P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.53 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.50 e $Å^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cu1—N1 | 1.907 (4) | Cu1—N4 | 1.883 (4) |
| Cu1—N2$^{i}$ | 1.891 (4) | Cu1—N5$^{ii}$ | 1.899 (4) |
| N1—Cu1—N4 | 177.4 (2) | N2$^{i}$—Cu1—N5$^{ii}$ | 178.6 (2) |

Symmetry codes: (i) $x+1, y, z$; (ii) $x-1, y, z$.

The *N*-heterocycle is disordered over two sites and was refined as two overlapping fused rings with a large number of restraints. The occupancy for each component is 0.5. For each, the pyridyl ring was refined as a rigid hexagon with 1.39 Å sides. For the five-membered ring portion of the $C_6H_4N(C)N$ fused ring, the C—N distances were restrained to within 1.35 (1) Å and the 1,3-related atoms were restrained to 2.18 (1) Å. Additionally, the distance between the pyridyl ring and the benzimidazolyl fused ring was restrained to 1.50 (1) Å. The vibrations of the C and N atoms were restrained to be nearly isotropic. All H atoms were treated as riding on their parent atoms (C—H = 0.93 Å), with $U_{iso}(H) = 1.2U_{eq}(C)$.

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

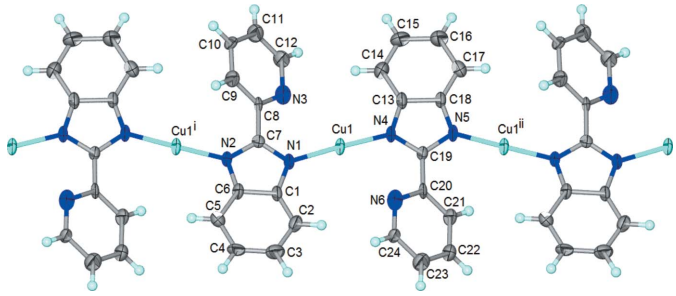



**Figure 1**
Plot of a portion of the polymeric chain structure in (I); displacement ellipsoids are drawn at the 50% probability level and H atoms as spheres of arbitrary radii. Only one of the two disordered components is shown. [Symmetry codes: (i) $1+x, y, z$; (ii) $x-1, y, z$.]

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