Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[copper(I)-μ-[2-(3-pyridyl)-benzimidazolato-κ^2N:N']]

Xiao-Chun Huang,[a] Wei Luo,[a] Yu-Feng Shen[a] and Seik Weng Ng[b]*

[a]Department of Chemistry, Shantou University, Shantou, Guangdong 515063, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603, Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

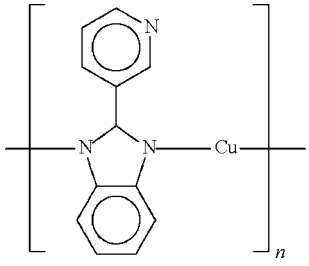
Received 27 June 2007; accepted 27 June 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.032; wR factor = 0.087; data-to-parameter ratio = 10.8.

The Cu atom in the title compound, $[Cu(C_{12}H_8N_3)]_n$, is linked to adjacent benzimidazolate N atoms in an almost linear CuN_2 geometry. The ligands link the Cu atoms into an infinite chain. The N atom and a C—H group of the pendant pyridine ring are disordered equally over two sites.

Related literature

For the structures of some copper(I) imidazolates, see Huang, Zhang & Chen (2004); Huang *et al.* (2005, 2006). For the synthesis of the ligand, see Huang, Zeng & Ng (2004). For the isomeric 2-pyridyl copper(I) complex, see Zeng *et al.* (2006).



Experimental

Crystal data

$[Cu(C_{12}H_8N_3)]$
M_r = 257.75
Orthorhombic, $Pna2_1$
a = 22.940 (3) Å
b = 11.055 (1) Å
c = 3.8050 (4) Å
V = 964.91 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.23 mm^{-1}
T = 295 (2) K
0.20 × 0.15 × 0.11 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.623, T_{max} = 0.791
3566 measured reflections
1568 independent reflections
1306 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.087
S = 1.05
1568 reflections
145 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack (1983), 620 Friedel pairs
Flack parameter: 0.04 (4)

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.866 (3)	Cu1—N2^{i}	1.866 (3)
N1—Cu1—N2^{i}	179.78 (16)		

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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: *publCIF* (Westrip, 2007).

The authors thank the Natural Science Foundation of Guangdong Province (grant Nos. 05300884 and 06027203), Shantou University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2460).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2002). *SMART* (Version 6.36A) and *SAINT* (Version 6.36A). Bruker AXS Inc., Madison, Winconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Huang, X.-C., Zeng, M.-H. & Ng, S. W. (2004). *Acta Cryst.* E**60**, o939–o940.
Huang, X.-C., Zhang, J.-P. & Chen, X.-M. (2004). *J. Am. Chem. Soc.* **126**, 13218–13219.
Huang, X.-C., Zhang, J.-P. & Chen, X.-M. (2006). *Cryst. Growth Des.* **6**, 1194–1198.
Huang, X.-C., Zhang, J.-P., Lin, Y.-Y. & Chen, X.-M. (2005). *Chem. Commun.* pp. 2232–2234.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Westrip, S. P. (2007). *publCIF*. In preparation.
Zeng, M.-H., Shen, X.-C. & Ng, S. W. (2006). *Acta Cryst.* E**62**, m2194–m2195.

supplementary materials

Acta Cryst. (2007). E**63**, m2041 [**doi:10.1107/S1600536807031455**]

catena-Poly[copper(I)-μ-[2-(3-pyridyl)benzimidazolato-κ^2N:N']]

X.-C. Huang, W. Luo, Y.-F. Shen and S. W. Ng

Comment

Imidazolates function as monoanionc μ_2-bridging ligands to copper(I) and silver(I), and the resulting compounds are single molecules or linear chains (Huang *et al.*, 2006). The copper derivatives exhibit more complicated structures, and this is brought about by a choice of reaction conditions. Copper compounds with a polygon motif (Huang, Zhang & Chen, 2004) as well as with triple helical chain motifs (Huang *et al.*, 2005) have been synthesized. The title compound is a pyridyl-substituted imidazolate; however, the pyridyl ring does not participate in bonding, so that the copper atom is linked only to the nitrogen atoms of two benzimidazolate anions in a linear geometry.

Experimental

2-(3-Pyridyl)-1*H*-benzimidazole was synthesized using a reported procedure (Huang, Zeng & Ng, 2004). A mixture of $Cu_2(OH)_2CO_3$ (0.110 g, 0.5 mmol), 2-(3-pyridyl)-1*H*-benzimidazole (0.195 g, 1.0 mmol), aqueous ammonia (25%, 5 ml) and methanol (2 ml) was placed in a 15-ml Teflon-lined bomb. The bomb was heated at 433 K for 80 h and then cooled to room temperature at a rate of 5 K h^{-1}. Pale-yellow needles of (I) were obtained in about 60% yield (based on the ligand). CH&N elemental analysis (calc/found) for $C_{12}H_8CuN_3$: C 56.03 (56.09), H 3.14(3.21), N 16.35% (16.28%).

Refinement

The pyridyl ring is disordered in the atoms at the *meta*-positions. These were refined as a 50:50 mixture of carbon and nitrogen. The pair of C/N atoms were restrained to the same site and also to have the same U^{ij} values. Hydrogen atoms were placed at calculated positions in the riding model approximation [C—H = 0.93 Å, U(H) = 1.2U_{eq}(C)].

Figures

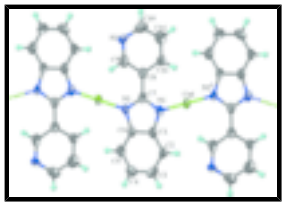


Fig. 1. **Figure 1**. View of a fragment of the chain motif in (I) showing 50% displacement ellipsoids for the non-hydrogen atoms. [Symmetry code (i): 3/2 + x, −1/2 -, z]

catena-Poly[copper(I)-μ-[2-(3-pyridyl)benzimidazolato- κ^2N:N']]

Crystal data

$[Cu(C_{12}H_8N_3)]$ F_{000} = 520

M_r = 257.75	D_x = 1.774 Mg m^{-3}
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2c -2n	Cell parameters from 1264 reflections
a = 22.940 (3) Å	θ = 3.2–27.9º
b = 11.055 (1) Å	μ = 2.23 mm^{-1}
c = 3.8050 (4) Å	T = 295 (2) K
V = 964.91 (18) Å^3	Rod, light yellow
Z = 4	0.20 × 0.15 × 0.11 mm

Data collection

Bruker APEX CCD diffractometer	1568 independent reflections
Radiation source: fine-focus sealed tube	1306 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.020
T = 295(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −25→25
T_{min} = 0.623, T_{max} = 0.791	k = −13→8
3566 measured reflections	l = −4→4

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.032	$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.087	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.05	$\Delta\rho_{max}$ = 0.48 e Å^{-3}
1568 reflections	$\Delta\rho_{min}$ = −0.23 e Å^{-3}
145 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 620 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.04 (4)
Secondary atom site location: difference Fourier map	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.74935 (2)	0.65062 (4)	0.5000 (4)	0.02952 (18)	
N1	0.72737 (15)	0.8039 (3)	0.3434 (9)	0.0286 (8)	
N2	0.72837 (15)	0.9975 (3)	0.1567 (9)	0.0261 (8)	
N3	0.91461 (16)	1.0027 (4)	0.3531 (12)	0.0364 (10)	0.50
C3'	0.91461 (16)	1.0027 (4)	0.3531 (12)	0.0364 (10)	0.50
H3'	0.9345	1.0707	0.4326	0.044*	0.50

C1	0.67013 (19)	0.8423 (3)	0.3150 (12)	0.0289 (10)	
C2	0.61824 (18)	0.7842 (3)	0.3838 (12)	0.0345 (11)	
H2	0.6177	0.7049	0.4656	0.041*	
C3	0.5674 (2)	0.8463 (4)	0.3283 (15)	0.0393 (12)	
H3	0.5319	0.8084	0.3725	0.047*	
C4	0.5677 (2)	0.9649 (4)	0.2074 (12)	0.0369 (11)	
H4	0.5325	1.0050	0.1732	0.044*	
C5	0.61899 (19)	1.0236 (4)	0.1378 (11)	0.0343 (10)	
H5	0.6191	1.1025	0.0529	0.041*	
C6	0.67062 (17)	0.9626 (3)	0.1972 (10)	0.0259 (9)	
C7	0.76014 (16)	0.9008 (4)	0.2484 (11)	0.0259 (9)	
C8	0.82406 (17)	0.8993 (4)	0.2412 (10)	0.0274 (9)	
C9	0.85672 (19)	0.9970 (4)	0.3604 (12)	0.0371 (11)	
H9	0.8367	1.0630	0.4518	0.045*	
C10	0.9427 (2)	0.9072 (4)	0.2275 (14)	0.0462 (12)	
H10	0.9832	0.9092	0.2209	0.055*	
C11	0.91465 (19)	0.8052 (4)	0.1062 (11)	0.0478 (12)	0.50
H11	0.9360	0.7402	0.0193	0.057*	0.50
N11'	0.91465 (19)	0.8052 (4)	0.1062 (11)	0.0478 (12)	0.50
C12	0.85523 (18)	0.8008 (4)	0.1152 (10)	0.0328 (11)	
H12	0.8357	0.7321	0.0373	0.039*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0323 (3)	0.0143 (3)	0.0419 (3)	−0.00030 (17)	−0.00202 (19)	0.0096 (3)
N1	0.033 (2)	0.0187 (18)	0.0344 (18)	0.0014 (16)	0.0004 (17)	0.0056 (17)
N2	0.0297 (19)	0.0132 (17)	0.0353 (16)	0.0004 (15)	−0.0029 (17)	0.0038 (16)
N3	0.024 (2)	0.025 (2)	0.060 (3)	−0.0050 (17)	−0.008 (2)	−0.002 (2)
C3'	0.024 (2)	0.025 (2)	0.060 (3)	−0.0050 (17)	−0.008 (2)	−0.002 (2)
C1	0.039 (3)	0.018 (2)	0.030 (2)	0.0008 (17)	0.000 (2)	0.0029 (19)
C2	0.035 (3)	0.019 (2)	0.049 (3)	−0.0057 (18)	0.000 (2)	0.0043 (18)
C3	0.033 (3)	0.036 (3)	0.048 (3)	−0.012 (2)	−0.006 (2)	0.006 (2)
C4	0.034 (3)	0.033 (3)	0.044 (3)	0.005 (2)	−0.004 (2)	−0.001 (2)
C5	0.044 (3)	0.020 (2)	0.039 (2)	0.004 (2)	−0.002 (2)	0.0056 (18)
C6	0.033 (3)	0.017 (2)	0.028 (2)	0.0013 (17)	0.001 (2)	0.0042 (18)
C7	0.034 (3)	0.015 (2)	0.0283 (17)	−0.0012 (17)	−0.001 (2)	0.0076 (16)
C8	0.034 (3)	0.020 (2)	0.0291 (19)	−0.0012 (19)	0.002 (2)	0.0063 (16)
C9	0.045 (3)	0.021 (2)	0.046 (2)	0.001 (2)	−0.002 (2)	0.003 (2)
C10	0.032 (3)	0.046 (3)	0.061 (3)	−0.008 (2)	−0.005 (3)	0.012 (3)
C11	0.050 (3)	0.038 (2)	0.055 (3)	0.005 (2)	0.000 (2)	0.005 (2)
N11'	0.050 (3)	0.038 (2)	0.055 (3)	0.005 (2)	0.000 (2)	0.005 (2)
C12	0.028 (3)	0.026 (2)	0.044 (3)	−0.0018 (18)	−0.001 (2)	0.0018 (19)

Geometric parameters (Å, °)

Cu1—N1	1.866 (3)	C3—H3	0.9300
Cu1—N2^{i}	1.866 (3)	C4—C5	1.370 (5)

N1—C7	1.357 (6)	C4—H4	0.9300
N1—C1	1.384 (5)	C5—C6	1.382 (5)
N2—C7	1.340 (5)	C5—H5	0.9300
N2—C6	1.388 (5)	C7—C8	1.467 (5)
N2—Cu1^{ii}	1.866 (3)	C8—C12	1.389 (6)
N3—C10	1.326 (6)	C8—C9	1.390 (5)
N3—C9	1.330 (5)	C9—H9	0.9300
C1—C2	1.378 (5)	C10—C11	1.378 (6)
C1—C6	1.404 (4)	C10—H10	0.9300
C2—C3	1.371 (6)	C11—C12	1.364 (6)
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.389 (5)	C12—H12	0.9300
N1—Cu1—N2^{i}	179.78 (16)	C6—C5—H5	120.9
C7—N1—C1	105.3 (3)	C5—C6—N2	131.6 (4)
C7—N1—Cu1	130.7 (3)	C5—C6—C1	120.5 (4)
C1—N1—Cu1	124.0 (3)	N2—C6—C1	107.8 (4)
C7—N2—C6	105.6 (3)	N2—C7—N1	113.4 (4)
C7—N2—Cu1^{ii}	131.1 (3)	N2—C7—C8	123.2 (4)
C6—N2—Cu1^{ii}	123.3 (3)	N1—C7—C8	123.4 (4)
C10—N3—C9	117.1 (4)	C12—C8—C9	116.4 (4)
C2—C1—N1	131.5 (4)	C12—C8—C7	122.0 (4)
C2—C1—C6	120.6 (4)	C9—C8—C7	121.6 (4)
N1—C1—C6	107.9 (4)	N3—C9—C8	124.6 (4)
C3—C2—C1	118.2 (4)	N3—C9—H9	117.7
C3—C2—H2	120.9	C8—C9—H9	117.7
C1—C2—H2	120.9	N3—C10—C11	123.0 (4)
C2—C3—C4	121.3 (4)	N3—C10—H10	118.5
C2—C3—H3	119.4	C11—C10—H10	118.5
C4—C3—H3	119.4	C12—C11—C10	119.2 (4)
C5—C4—C3	121.1 (4)	C12—C11—H11	120.4
C5—C4—H4	119.5	C10—C11—H11	120.4
C3—C4—H4	119.5	C11—C12—C8	119.7 (4)
C4—C5—C6	118.3 (4)	C11—C12—H12	120.2
C4—C5—H5	120.9	C8—C12—H12	120.2
C7—N1—C1—C2	−178.5 (5)	Cu1^{ii}—N2—C7—N1	−178.8 (3)
Cu1—N1—C1—C2	−0.7 (7)	C6—N2—C7—C8	179.7 (4)
C7—N1—C1—C6	0.8 (5)	Cu1^{ii}—N2—C7—C8	0.2 (6)
Cu1—N1—C1—C6	178.6 (3)	C1—N1—C7—N2	−0.9 (5)
N1—C1—C2—C3	−179.7 (5)	Cu1—N1—C7—N2	−178.6 (3)
C6—C1—C2—C3	1.1 (6)	C1—N1—C7—C8	−180.0 (4)
C1—C2—C3—C4	−0.2 (7)	Cu1—N1—C7—C8	2.4 (6)
C2—C3—C4—C5	0.3 (7)	N2—C7—C8—C12	−137.8 (4)
C3—C4—C5—C6	−1.2 (6)	N1—C7—C8—C12	41.1 (6)
C4—C5—C6—N2	−179.2 (4)	N2—C7—C8—C9	42.1 (6)
C4—C5—C6—C1	2.0 (6)	N1—C7—C8—C9	−138.9 (4)
C7—N2—C6—C5	−179.0 (4)	C10—N3—C9—C8	−1.0 (8)
Cu1^{ii}—N2—C6—C5	0.5 (6)	C12—C8—C9—N3	1.7 (7)

C7—N2—C6—C1	−0.1 (4)	C7—C8—C9—N3	−178.2 (4)
Cu1^{ii}—N2—C6—C1	179.4 (3)	C9—N3—C10—C11	0.3 (8)
C2—C1—C6—C5	−2.0 (6)	N3—C10—C11—C12	−0.2 (8)
N1—C1—C6—C5	178.6 (4)	C10—C11—C12—C8	0.9 (7)
C2—C1—C6—N2	178.9 (4)	C9—C8—C12—C11	−1.6 (7)
N1—C1—C6—N2	−0.4 (4)	C7—C8—C12—C11	178.4 (4)
C6—N2—C7—N1	0.7 (5)		

Symmetry codes: (i) −*x*+3/2, *y*−1/2, *z*+1/2; (ii) −*x*+3/2, *y*+1/2, *z*−1/2.

Fig. 1