Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[(pyrazino[2,3-*f*][1,10]phenanthroline)copper(**I**)]-μ_2-chloro]

Guang-Bo Che,* Zhan-Lin Xu and Chun-Bo Liu

Department of Chemistry, Jilin Normal University, Siping 136000, People's Republic of China

Correspondence e-mail:
guangbochejl@yahoo.com

Received 19 May 2006
Accepted 19 May 2006

Key indicators

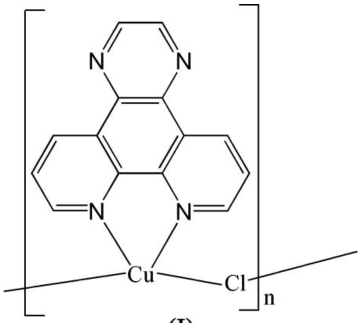
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.039
wR factor = 0.103
Data-to-parameter ratio = 14.8

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

In the title compound, $[\mathrm{CuCl(C_{14}H_8N_4)}]_n$, the central $\mathrm{Cu^I}$ ion displays a distorted tetrahedral geometry, coordinated by two $\mathrm{Cl^-}$ ions and two N atoms from a bidentate pyrazino[2,3-*f*]-[1,10]phenanthroline (PyPhen) ligand. Each $\mathrm{Cl^-}$ ion bridges two $\mathrm{Cu^I}$ atoms, forming a zigzag chain structure. Cu and Cl have site symmetry 2; the complete PyPhen molecule is generated by twofold symmetry.

Comment

Inorganic–organic coordination polymers based on $\mathrm{Cu^I}$ halides and aromatic nitrogen-donor ligands have been attracting increasing interest (Ford *et al.*, 1999). Previous results have shown that $\mathrm{Cu^I}$ halides can be combined with monodentate nitrogen-donor ligands, producing a wide array of structural types (Ohi *et al.*, 2005; Wang *et al.*, 2005). However, $\mathrm{Cu^I}$ halides with chelating bidentate nitrogen-donor ligands have rarely been investigated (Haddad & Willett, 2001). The 1,10-phenanthroline (Phen) ligand has been widely used to build novel supramolecular architectures through aromatic π–π interactions (Chen & Liu, 2002), while an important derivative of Phen, pyrazino[2,3-*f*][1,10]-phenanthroline (PyPhen), was recently used to synthesize coordination polymers (Che, 2006). We selected the chloride ion as a linker and PyPhen as a secondary chelating ligand, generating a new $\mathrm{Cu^I}$ coordination polymer, [CuCl(PyPhen)], (I), which is reported here.



(I)

The central $\mathrm{Cu^I}$ ion (site symmetry 2) in (I) displays a distorted tetrahedral geometry, coordinated (Table 1) by two $\mathrm{Cl^-}$ ions and two N atoms from PyPhen (Fig. 1). The complete PyPhen molecule is built up by a twofold axis that bisects the C4—C4$^{\mathrm{i}}$, C6—C6$^{\mathrm{i}}$ and C7—C7$^{\mathrm{i}}$ bonds [symmetry code: (i) $1-x, y, \frac{1}{2}-z$]. Each $\mathrm{Cl^-}$ ion (site symmetry 2) bridges two $\mathrm{Cu^I}$ atoms, generating a distinctive zigzag chain structure (Fig. 2) that propagates along [100]. The PyPhen ligands are thus attached to one side of a single-stranded chain.

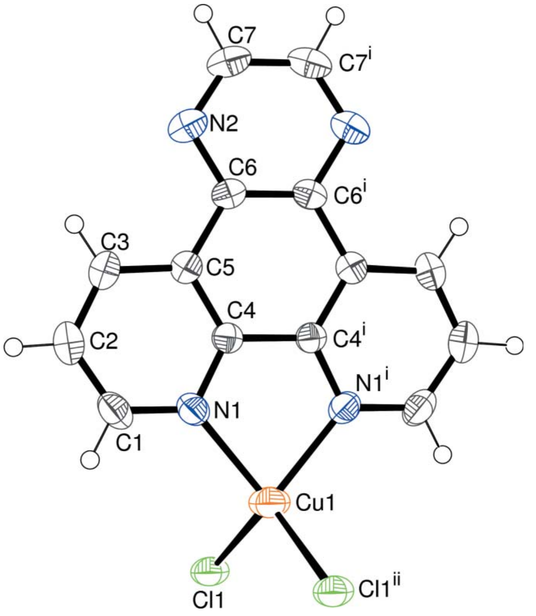


Figure 1
The asymmetric unit of (I), together with further atoms to complete the Cu^I coordination and the PyPhen ligand. Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms). [Symmetry codes: (i) $1 - x, y, \frac{1}{2} - z$; (ii) $x - 1, y, z$.]

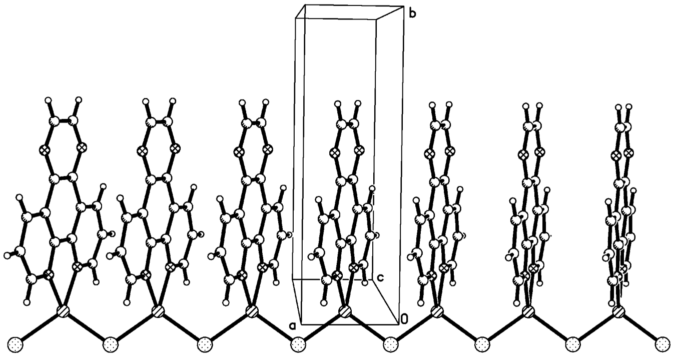


Figure 2
View of the single-chain polymeric structure of (I).

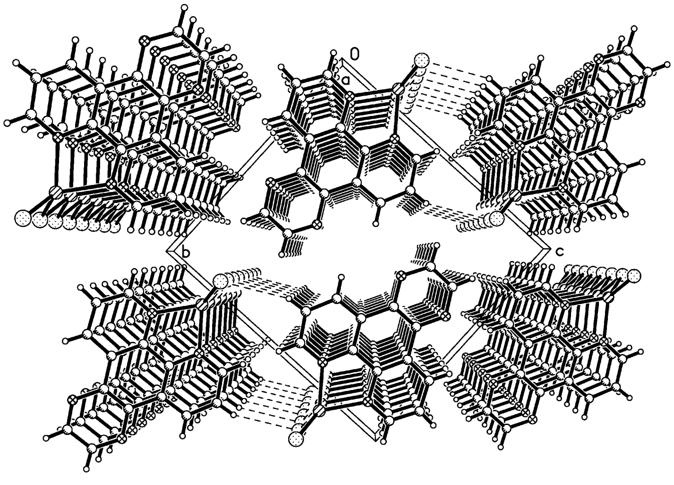


Figure 3
View of the packing of (I), with C—H$\cdots$Cl interactions shown as dashed lines.

There are π–π stacking interactions with a π–π stacking distance of 3.55 Å between PyPhen ligands in the same single chain. A long inter-chain C—H$\cdots$Cl interaction (Table 2) may also help to consolidate the crystal packing (Fig. 3).

Experimental

The PyPhen ligand was synthesized according to the literature method of Dickeson & Summers (1970). Compound (I) was hydrothermally synthesized under autogenous pressure: a mixture of PyPhen, $CuCl_2$ and water in a molar ratio of 2:1:5000 was sealed in a Teflon-lined autoclave and heated to 453 K for 3 d. Upon cooling and opening the bomb, orange plates and slabs of (I) were obtained (45% yield based on Cu).

Crystal data

$[CuCl(C_{14}H_8N_4)]$
$M_r = 331.23$
Monoclinic, $P2/c$
$a = 3.7354$ (7) Å
$b = 12.099$ (2) Å
$c = 13.129$ (3) Å
$\beta = 91.33$ (3)°
$V = 593.2$ (2) Å^3

$Z = 2$
$D_x = 1.854$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 2.06$ mm^{-1}
$T = 292$ (2) K
Slab, orange
0.31 × 0.28 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.539$, $T_{max} = 0.679$

5650 measured reflections
1358 independent reflections
1067 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.103$
$S = 1.08$
1358 reflections
92 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 0.4657P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—Cu1	2.3013 (7)	Cu1—N1	2.094 (2)
N1^i—Cu1—N1	79.52 (13)	N1—Cu1—Cl1	106.22 (7)
N1—Cu1—Cl1^{ii}	128.23 (7)	Cl1^{ii}—Cu1—Cl1	108.50 (5)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2$\cdots$Cl1^{iii}	0.93	2.87	3.720 (4)	153

Symmetry code: (iii) $-x + 2, -y, -z$.

All H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997);

Acta Cryst. (2006). E**62**, m1370–m1372 Che *et al.* • $[CuCl(C_{14}H_8N_4)]$ **m1371**

program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

The authors thank Jilin Normal University for supporting this work.

References

Che, G.-B. (2006). *Acta Cryst.* E**62**, m1244–m1246.

Chen, X.-M. & Liu, G.-F. (2002). *Chem. Eur. J.* **8**, 4811–4817.

Dickeson, J. E. & Summers, L. A. (1970). *Aust. J. Chem.* **23**, 1023–1027.

Ford, P. C., Cariati, E. & Bourassa, J. (1999). *Chem. Rev.* **99**, 3625–3647.

Haddad, S. & Willett, R. D. (2001). *Inorg. Chem.* **40**, 809–811.

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.

Ohi, H., Tachi, Y., Kunimoto, T. & Itoh, S. (2005). *Dalton Trans.* pp. 3146–3147.

Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.

Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Góttingen, Germany.

Wang, X. Q., Cheng, J. K., Wen, Y. H., Zhang, J., Li, Z. J. & Yao, Y. G. (2005). *Inorg. Chem. Commun.* **8**, 897–899.

m1372 Che *et al.* • [CuCl($C_{14}H_8N_4$)] *Acta Cryst.* (2006). E**62**, m1370–m1372