

(2,2'-Bipyridine- κ^2N,N')dichlorocopper(II)Yan-Qin Wang,* Wen-Hua Bi,
Xing Li and Rong CaoState Key Laboratory of Structural Chemistry,
Fujian Institute of Research on the Structure of
Matter, Fuzhou, Fujian 350002, People's
Republic of ChinaCorrespondence e-mail:
yqwang@ms.fjirsm.ac.cn

Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.011\text{ \AA}$
 R factor = 0.055
 wR factor = 0.158
Data-to-parameter ratio = 13.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.The title compound, $[\text{CuCl}_2(\text{C}_{10}\text{H}_8\text{N}_2)]$, has twofold symmetry and the coordination geometry around the Cu^{II} atom is distorted square-planar. There are weak intermolecular $\text{Cu} \cdots \text{Cl}$ interactions, forming a chain structure in the crystal.Received 13 May 2004
Accepted 24 May 2004
Online 29 May 2004

Comment

The title compound, (I), is a simple coordination complex of Cu and 2,2'-bipyridine (bpy).

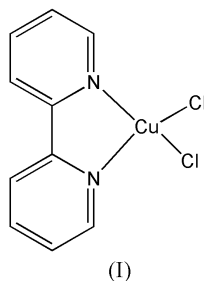
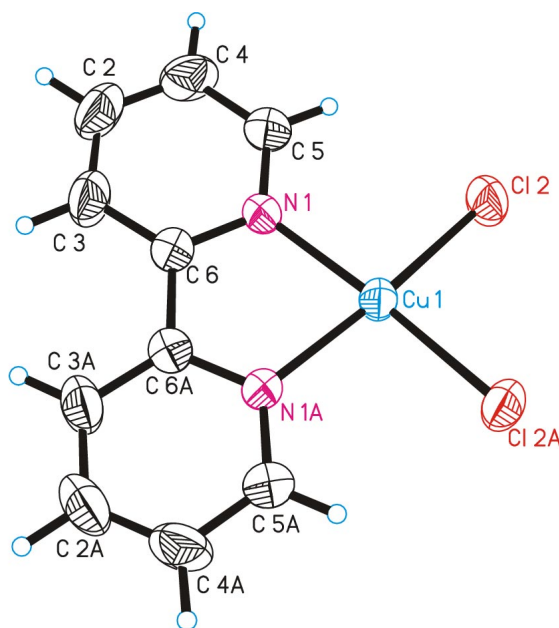
The central Cu atom in (I) lies on a twofold axis, and is coordinated by two N atoms from the bpy ligand and two Cl atoms, which form a distorted square (Fig. 1 and Table 1). The $\text{N1}-\text{C6}-\text{C6}^{\text{ii}}-\text{N1}^{\text{ii}}$ torsion angle of the bpy ligand is $5.5(3)^\circ$ [symmetry code: (ii) $-x, y, \frac{1}{2} - z$].

Figure 1

A view of the molecular structure of (I), showing 50% probability displacement ellipsoids. [Symmetry code: (A) $-x, y, \frac{1}{2} - z$.]

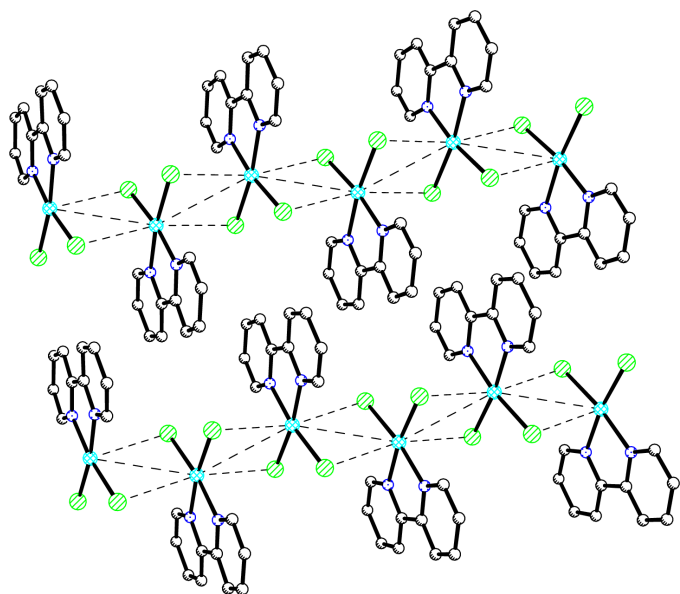


Figure 2
The chain structure in the crystal of (I). H atoms have been omitted for clarity.

Neighbouring molecules are connected by weak $\text{Cu1} \cdots \text{Cl2}^i$ interactions of 3.047 (3) Å, forming a chain structure (Fig. 2) [symmetry code: (i) $-x, 1 - y, -z$]. The $\text{Cu} \cdots \text{Cu}^i$ distance in the chain is 3.811 (4) Å.

Experimental

Compound (I) was produced unexpectedly. $[\text{Cu}(\text{bpy})\text{-}(\text{dien})\text{Cl}]\text{Cl}\cdot 3\text{H}_2\text{O}$ (0.136 g, 0.3 mmol) and 1,3,5-benzenetricarboxylic acid (0.021 g, 0.1 mmol) were dissolved in water (20 ml). To this solution, two drops of 1 M NaOH were added. The final solution was sealed in a 25 ml Teflon-lined stainless steel bomb and heated to 433 K for 4 d, and then cooled to room temperature. A clear green solution was obtained and green prismatic crystals of (I) were collected by evaporation of the solution, with a yield of 35.6%.

Crystal data

$[\text{CuCl}_2(\text{C}_{10}\text{H}_8\text{N}_2)]$
 $M_r = 290.63$
 Monoclinic, $C2/c$
 $a = 17.08$ (5) Å
 $b = 8.95$ (2) Å
 $c = 7.23$ (2) Å
 $\beta = 112.52$ (3)°
 $V = 1021$ (5) Å³
 $Z = 4$

$D_x = 1.890$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 1248 reflections
 $\theta = 3.6\text{--}25.0^\circ$
 $\mu = 2.62$ mm⁻¹
 $T = 293$ (2) K
 Prism, green
 $0.32 \times 0.24 \times 0.16$ mm

Data collection

Rigaku Mercury70 CCD
 diffractometer (2×2 bin mode)
 ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.343$, $T_{\text{max}} = 0.657$
 2958 measured reflections

904 independent reflections
 691 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.052$
 $\theta_{\text{max}} = 25.0^\circ$
 $h = -18 \rightarrow 20$
 $k = -9 \rightarrow 10$
 $l = -8 \rightarrow 8$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.055$
 $wR(F^2) = 0.158$
 $S = 1.05$
 904 reflections
 69 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0887P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.45$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.73$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1—N1	2.024 (6)	Cu1—Cl2 ⁱ	3.047 (3)
Cu1—Cl2	2.254 (4)		
N1—Cu1—N1 ⁱⁱ	80.5 (3)	Cl2 ⁱⁱ —Cu1—Cl2	93.0 (2)
N1—Cu1—Cl2 ⁱⁱ	172.16 (14)	N1—Cu1—Cl2 ⁱ	84.8 (3)
N1—Cu1—Cl2	93.4 (2)	Cl2—Cu1—Cl2 ⁱ	89.3 (4)

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

The relatively large s.u. values of the lattice constants may be due to the crystal itself and the optical process. The positions of all H atoms were generated geometrically ($\text{C—H} = 0.97$ Å) and they were allowed to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$.

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *ORTEP3* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Natural Science Foundation of China and the Natural Science Foundation of Fujian Province.

References

- Burnett, M. N. & Johnson, C. K. (1996). *ORTEP3*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Molecular Structure Corporation & Rigaku (2000). *CrystalClear*. Version 1.36. MSC, 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA, and Rigaku Corporation, 3-9-12 Akishima, Tokyo, Japan.
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.