Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Dichloro[*N*,*N*-dimethyl-*N*′-(2-pyridylmethylidene)-ethane-1,2-diamine]copper(II)

Wen-Bing Yuan and Qi Zhang*

Hainan Provincial Key Lab of Fine Chemicals, Hainan University, Hainan 570228, People's Republic of China

Correspondence e-mail:
zhangqi_hainu@163.com

Received 18 August 2005
Accepted 24 August 2005
Online 31 August 2005

Key indicators

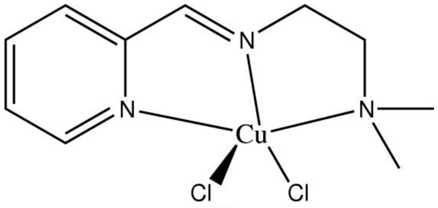
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.025
wR factor = 0.060
Data-to-parameter ratio = 20.2

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

The title complex, $[CuCl_2(C_{10}H_{15}N_3)]$, is a mononuclear copper(II) compound. The Cu^{II} atom has a distorted square-pyramidal coordination. In the basal plane, the Cu atom is coordinated by three N atoms of the Schiff base ligand, and by one terminal Cl atom. The apical position is occupied by another Cl atom.

Comment

For the past few years there has been a burgeoning effort to identify the biological role of copper, primarily through techniques associated with the interface of biology/biochemistry/coordination chemistry (Collinson & Fenton, 1996; Hossain *et al.*, 1996; Tarafder *et al.*, 2002). It appears that the biological role of copper is primarily in redox reactions and as a biological catalyst, although much remains to be understood (Musie *et al.*, 2003; García-Raso *et al.*, 2003). An extensive effort has been made to prepare and characterize a variety of copper(II) coordination complexes in an attempt to model the physical and chemical behaviour of copper-containing enzymes (Reddy *et al.*, 2000). The peculiarity of copper lies in its ability to form complexes with coordination numbers four and five, as well as six (Ray *et al.*, 2003; Arnold *et al.*, 2003; Raptopoulou *et al.*, 1998). As part of our investigations in this area we report here a new mononuclear copper(II) complex, (I) (Fig. 1).



(I)

The Cu^{II} atom has a square-pyramidal geometry. In the basal plane, the Cu^{II} atom is coordinated by three N atoms of the Schiff base and by one Cl atom. The apical position is occupied by another terminal Cl atom. A severe distortion of the square pyramid is revealed by the bond angles between the apical and basal donor atoms (Table 1). A view of the molecular packing is shown in Fig. 2.

Experimental

N,*N*-Dimethylethane-1,2-diamine (0.1 mmol, 8.8 mg), 2-pyridylaldehyde (0.1 mmol, 10.7 mg) and $CuCl_2\cdot 4H_2O$ (0.1 mmol, 20.7 mg) were dissolved in methanol (15 ml). The mixture was stirred at 328 K for 20 min and filtered. The filtrate was kept in air for 21 d, and blue block crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

Crystal data

$[CuCl_2(C_{10}H_{15}N_3)]$
$M_r = 311.69$
Triclinic, $P\overline{1}$
$a = 7.303$ (1) Å
$b = 8.009$ (1) Å
$c = 11.995$ (1) Å
$\alpha = 100.181$ (1)°
$\beta = 101.946$ (1)°
$\gamma = 100.855$ (1)°
$V = 656.90$ (13) Å^3
$Z = 2$
$D_x = 1.576$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4455 reflections
$\theta = 2.7$–28.2°
$\mu = 2.05$ mm^{-1}
$T = 298$ (2) K
Block, blue
0.22 × 0.10 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.662$, $T_{max} = 0.853$
7629 measured reflections
2972 independent reflections
2774 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 27.5°$
$h = -9 \rightarrow 9$
$k = -10 \rightarrow 10$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.060$
$S = 1.09$
2972 reflections
147 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0265P)^2 + 0.0926P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	2.104 (2)	Cu1—Cl2	2.257 (1)
Cu1—N1	2.236 (2)	Cu1—N3	2.275 (2)
Cu1—Cl1	2.256 (1)		
N2—Cu1—N1	74.25 (6)	Cl1—Cu1—Cl2	114.01 (2)
N2—Cu1—Cl1	132.19 (4)	N2—Cu1—N3	76.84 (6)
N1—Cu1—Cl1	95.85 (4)	N1—Cu1—N3	150.35 (6)
N2—Cu1—Cl2	113.68 (4)	Cl1—Cu1—N3	98.64 (4)
N1—Cu1—Cl2	98.29 (4)	Cl2—Cu1—N3	99.20 (4)

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) values of 1.2 or 1.5 times U_{eq}(parent atom).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to Hainan University for financial support.

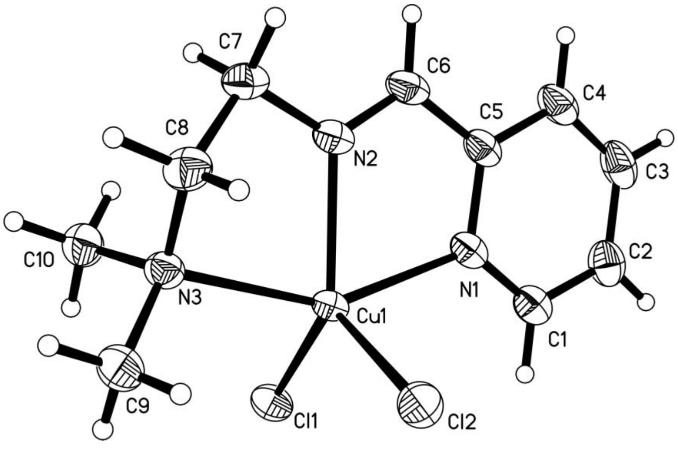


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

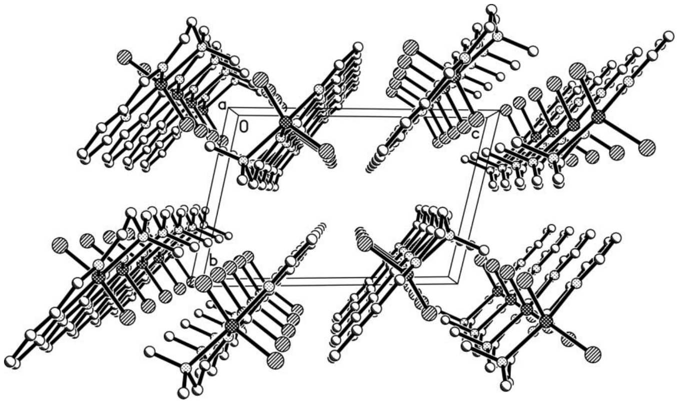


Figure 2
The crystal packing of (I), viewed down the *a* axis. H atoms have been omitted.

References

Arnold, P. J., Davies, S. C., Durrant, M. C., Griffiths, D. V., Hughes, D. L. & Sharpe, P. C. (2003). *Inorg. Chim. Acta*, **348**, 143–149.

Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.

Collinson, S. R. & Fenton, D. E. (1996). *Coord. Chem. Rev.* **148**, 19–40.

García-Raso, Á., Fiol, J. J., López-Zafra, A., Castro, J. A., Cabrero, A., Mata, I. & Molins, E. (2003). *Polyhedron*, **22**, 403–409.

Hossain, M. E., Alam, M. N., Begum, J., Ali, M. A., Nazimuddin, M., Smith, F. E. & Hynes, R. C. (1996). *Inorg. Chim. Acta*, **249**, 207–213.

Musie, G. T., Li, X. & Powell, D. R. (2003). *Inorg. Chim. Acta*, **348**, 69–74.

Raptopoulou, C. P., Papadopoulos, A. N., Malamatari, D. A., Ioannidis, E., Moisidis, G., Terzis, A. & Kessissoglou, D. P. (1998). *Inorg. Chim. Acta*, **272**, 283–290.

Ray, M. S., Bhattacharya, R. B., Chaudhuri, S., Righi, L., Bocelli, G., Mukhopadhyay, G. & Ghosh, A. (2003). *Polyhedron*, **22**, 617–624.

Reddy, P. A. N., Datta, R. & Chakravarty, A. R. (2000). *Inorg. Chem. Commun.* **3**, 322–324.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

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

Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

Tarafder, M. T. H., Jin, K. T., Crouse, K. A., Ali, A. M., Yamin, B. M. & Fun, H.-K. (2002). *Polyhedron*, **21**, 2547–2554.