Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Aquadichloro(2,9-dimethyl-1,10-phenanthroline-κ^2N,N')copper(II)

Pascale Lemoine,[a]* Bernard Viossat[a,b] and Jean-Claude Daran[c]

[a]Laboratoire de Cristallographie et RMN Biologiques, UMR 8015 CNRS, Faculté des Sciences Pharmaceutiques et Biologiques de Paris V, 4 Avenue de l'Observatoire, 75270 Paris Cedex 06, France, [b]Laboratoire de Chimie Générale, Faculté de Médecine et de Pharmacie, 34 rue du Jardin des Plantes, BP199, 86005 Poitiers Cedex, France, and [c]Laboratoire de Chimie de Coordination, UPR 8241 CNRS, 205 route de Narbonne 31077 Toulouse Cedex 04, France

Correspondence e-mail:
lemoine@pharmacie.univ-paris5.fr

Received 12 November 2002
Accepted 2 December 2002
Online 19 December 2002

The crystal structure of the title compound, $[CuCl_2(C_{14}H_{12}N_2)(H_2O)]$, previously reported by Preston & Kennard [*J. Chem. Soc. A* (1969). pp. 2955–2958], has been redetermined. The recognition of an inversion twin allowed a much better refinement.

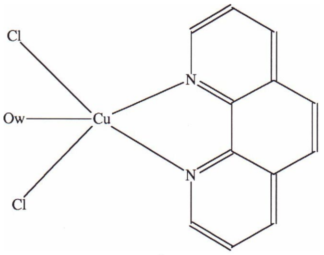
Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.004 Å
R factor = 0.017
wR factor = 0.046
Data-to-parameter ratio = 11.1

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

Comment

The asymmetric unit of the title compound, (I), contains one monomeric five-coordinate copper complex. The Cu atom is coordinated by one 2,9-dimethyl-1,10-phenanthroline (neocuproine) ligand *via* both N atoms, two Cl^- anions and to one water molecule. The complex exhibits a distorted square pyramidal geometry about the copper(II) atom, with the apical position occupied by atom N10 from the neocuproine ligand. The Cu atom is displaced by 0.3074 (6) Å out of the basal plane defined by atoms N1, Cl1, Cl2 and *O*W1. An alternative description of this molecule would be trigonal bipyramidal, with atoms N1 and *O*W1 in axial positions [*O*W1 Cu1 N1 171.50 (8)°; the Cu atom is 0.0327 (3) Å out of the equatorial plane]. However, analysis of the τ factor, proposed by Addison & Rao (1984) for five-coordinate copper complexes, makes the description as distorted square pyramidal more correct, with a τ value of 0.267 (τ square pyramidal = 0.0, τ trigonal bipyramidal = 1.0).



(I)

The crystal packing is characterized by two hydrogen bonds [*O*W–H*W*1···Cl1^{i}: 3.088 (2) Å, 159 (3)°; *O*W–H*W*2···Cl2^{ii} 3.029 (2) Å, 162 (3)°; symmetry codes: (i) $-x$, $y+\frac{1}{2}$, $-z$; (ii) $-x$, $y-\frac{1}{2}$, $-z$]; these interactions result in chains parallel to the *b* axis. The neocuproine least-squares planes are linked by π-π stacking interactions, related, in pairs, by the twofold screw axis, with an average spacing of 3.153 Å (symmetry code: $1-x$, $-\frac{1}{2}+y$, $1-z$).

Experimental

The title compound was synthesized according to Preston & Kennard (1969). Green parallelepiped crystals were obtained by recrystallization from methanol.

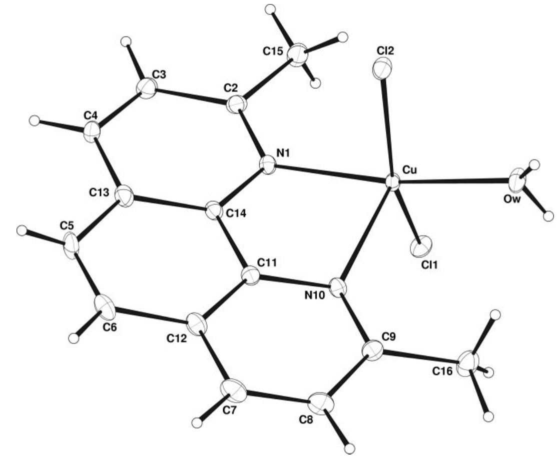


Figure 1
Perspective view of the asymmetric unit, showing the atomic numbering. Displacement ellipsoids are at the 50% probability level.

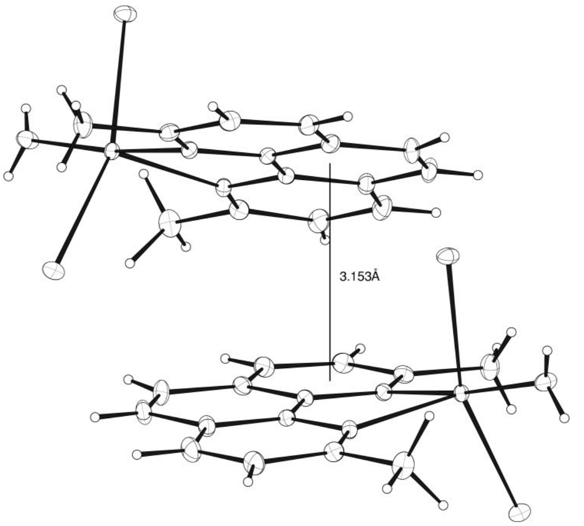


Figure 2
The π–π-stacking interactions between neocuproine ligands.

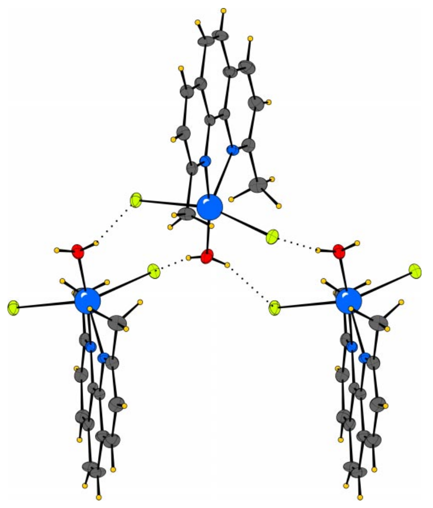


Figure 3
The molecular packing, showing chains formed by hydrogen bonds.

Crystal data

$[CuCl_2(C_{14}H_{12}N_2)(H_2O)]$
$M_r = 360.71$
Monoclinic, $P2_1$
$a = 9.462$ (1) Å
$b = 8.093$ (1) Å
$c = 9.823$ (1) Å
$\beta = 105.38$ (1)°
$V = 725.3$ (1) Å^3
$Z = 2$
$D_x = 1.652$ Mg m^{-3}
$D_m = 1.63$ (2) Mg m^{-3}
D_m measured by flotation in $CCl_4/C_2H_4Br_2$
Mo $K\alpha$ radiation
Cell parameters from 5681 reflections
$\theta = 2.2$–26.1°
$\mu = 1.87$ mm^{-1}
$T = 180$ (2) K
Parallelepiped, green
0.30 × 0.25 × 0.20 mm

Data collection

Stoe IPDS diffractometer
φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996; Blessing, 1995)
$T_{\min} = 0.511$, $T_{\max} = 0.569$
5663 measured reflections
2499 independent reflections
2425 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.018$
$\theta_{\max} = 26.1$°
$h = -10 \rightarrow 10$
$k = -9 \rightarrow 9$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.017$
$wR(F^2) = 0.046$
$S = 1.05$
2499 reflections
225 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.27$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}
Absolute structure: Flack (1983), 951 Friedel pairs
Flack parameter = 0.538 (8)

Table 1
Selected geometric parameters (Å, °).

Cu—O*W*	1.9582 (15)	Cu—Cl2	2.3017 (5)
Cu—N1	1.9911 (15)	Cu—Cl1	2.3026 (6)
Cu—N10	2.230 (2)		
O*W*—Cu—N1	171.44 (7)	N1—Cu—Cl1	94.84 (5)
O*W*—Cu—N10	107.34 (7)	N10—Cu—Cl1	103.92 (5)
N1—Cu—N10	79.98 (7)	Cl2—Cu—Cl1	155.36 (2)
O*W*—Cu—Cl2	87.57 (5)	C2—N1—Cu	123.98 (15)
N1—Cu—Cl2	86.68 (6)	C14—N1—Cu	114.81 (11)
N10—Cu—Cl2	100.57 (5)	C9—N10—Cu	133.46 (16)
O*W*—Cu—Cl1	87.77 (6)	C11—N10—Cu	107.36 (14)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O*W*—H*W*1···Cl1^{i}	0.77 (4)	2.36 (4)	3.0882 (17)	159 (3)
O*W*—H*W*2···Cl2^{ii}	0.75 (4)	2.31 (4)	3.0286 (17)	162 (3)

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

H atoms were located from difference Fourier maps and freely refined; a common displacement parameter was refined for all H atoms. The refinement of the Flack (1983) parameter [$x = 0.538$ (8)] clearly indicates the occurrence of an inversion twin.

Data collection: *IPDS Software* (Stoe & Cie, 1996); cell refinement: *IPDS Software*; data reduction: *XRED* (Stoe & Cie, 1996); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *WinGX* (Version 1.63.02; Farrugia, 1999).

m18 Pascale Lemoine *et al.* • $[CuCl_2(C_{14}H_{12}N_2)(H_2O)]$ *Acta Cryst.* (2003). E**59**, m17–m19

References

Addison, A. W. & Rao, T. N. (1984). *J. Chem. Soc. Dalton Trans.* pp. 1349–1356.

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Preston, H. S. & Kennard, C. H. L. (1969). *J. Chem. Soc.* A, pp. 2955–2958.

Stoe & Cie (1996). *IPDS Manual* (Version 2.75) and *X-RED* (Revision 1.08). Stoe & Cie, Darmstadt, Germany.

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

Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.

Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.

Acta Cryst. (2003). E**59**, m17–m19 Pascale Lemoine *et al.* • $[CuCl_2(C_{14}H_{12}N_2)(H_2O)]$ **m19**