Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Dichloro[2-(2-furyl)-1*H*-benzimidazole-κN^3]-copper(II)

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
R factor = 0.023
wR factor = 0.068
Data-to-parameter ratio = 13.5

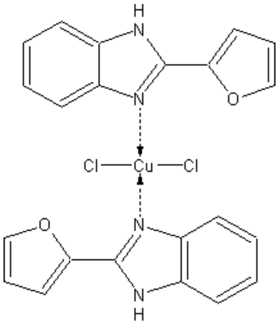
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 15 November 2004
Accepted 25 November 2004
Online 18 December 2004

In the title compound, $[CuCl_2(C_{11}H_8N_2O)_2]$, the Cu^{II} atom is coordinated by two N and two Cl atoms in a centrosymmetric square-planar geometry. Intermolecular N—H···Cl hydrogen bonds link the molecules into a two-dimensional network.

Comment

Schiff base ligands are widely used in the synthesis of metal complexes (Coles *et al.*, 1998). During the synthesis of Schiff base ligands, several novel cyclized ligands, such as 2-(2-hydroxyphenyl)benzimidazole (HPBI) (Rodrigo *et al.*, 2000), were obtained accidentally by the reaction of 1,2-phenylenediamine and aromatic aldehydes. In the past, only a few metal complexes with cyclized ligands have been studied crystallographically (Li *et al.*, 2002; Robert *et al.*, 1998). To our knowledge, no crystal structures of metal complexes with a cyclized ligand formed by furaldehyde and 1,2-phenylenediamine have been reported to date. In a continuation of our study of cyclized ligands and their metal complexes, we report here the crystal structure of the title complex, (I), a new mononuclear copper(II) complex, (I) (Fig. 1).



(I)

The geometric parameters of (I) are listed in Table 1. Complex (I) is centrosymmetric; the Cu atom is four-coordinated in a square-planar geometry by two chloride anions and two monodentate 2-(2-furyl)-1*H*-benzimidazole ligands through non-H-bonded N atoms. The Cu—N1 and Cu—Cl bond distances are 1.9756 (14) and 2.2852 (5) Å, respectively, which are similar to those found previously in the four-coordinated copper(II) complexes $[CuCl_2(mtz)]$ [mtz is 5-methyl-1,3,4-thiadiazole; average 2.058 (3) and 2.268 (1) Å; Song *et al.*, 2003] and $[CuCl_2(4,7\text{-phenanthroline})]$ [average 1.985 (3) and 2.2552 (9) Å; Barnett *et al.*, 2003]. In the title complex, the O atom of the furyl ring does not coordinate to the Cu atom [Cu···O = 2.971 (2) Å], and a similar situation was observed in the complex [*N*,*N*′-bis(2-furylmethylene)ethylenediamine]dichlorozinc(II) (Wang *et al.*, 2004). Intermolecular N—H···Cl

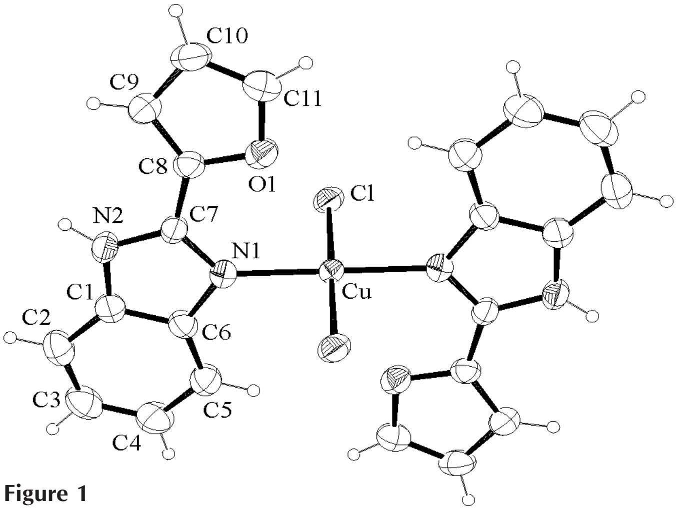


Figure 1
View of the molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by $(-x, 2-y, 2-z)$.

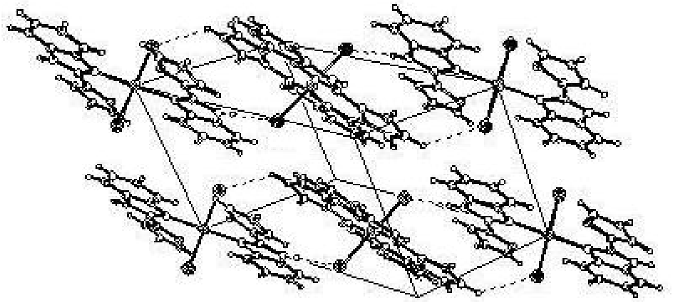


Figure 2
Crystal packing of (I). The intermolecular N—H···Cl hydrogen bonds are shown as dashed lines.

hydrogen bonds (Table 2) link the molecules into a two-dimensional network (Fig. 2).

Experimental

All reagents used were of analytical grade from commercial sources and used without further purification. To a solution of 1,2-phenylenediamine in absolute methanol was added furaldehyde (ratio of 1:2). The mixture was stirred for 30 min at room temperature and then $CuCl_2$ in absolute methanol (ratio 1:1 *M*:*L*) was added slowly with stirring to the resultant bright yellow solution. The solution turned brown–red during addition, the precipitate was filtered off and red single crystals suitable for X-ray analysis were obtained by slow evaporation of the filtrate after a few days.

Crystal data

$[CuCl_2(C_{11}H_8N_2O)_2]$
$M_r = 502.83$
Monoclinic, $P2_1/c$
$a = 8.8112$ (9) Å
$b = 14.1852$ (14) Å
$c = 9.1367$ (9) Å
$\beta = 111.8670$ (10)°
$V = 1059.82$ (18) Å^3
$Z = 2$

$D_x = 1.576$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 2608 reflections
$\theta = 2.5$–29.0°
$\mu = 1.31$ mm^{-1}
$T = 273$ (2) K
Block, red
0.35 × 0.30 × 0.28 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.554$, $T_{max} = 0.693$
5326 measured reflections

1912 independent reflections
1728 reflections with $I > 2\sigma(I)$
$R_{int} = 0.012$
$\theta_{max} = 25.3°$
$h = -10 \rightarrow 10$
$k = -17 \rightarrow 14$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.069$
$S = 1.11$
1912 reflections
142 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0381P)^2 + 0.1747P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—N1	1.9756 (14)	Cu—Cl	2.2852 (5)
N1—Cu—Cl^i	90.25 (5)	N1—Cu—Cl	89.75 (5)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···Cl^{ii}	0.86	2.33	3.1731 (17)	168

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

All H atoms were treated as riding, with C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$, N—H = 0.86 Å and $U_{iso}(H) = 1.2U_{eq}(N)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT* and *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

We acknowledge the support of the National Natural Science Foundation of China and the Provincial Natural Foundation of Shaanxi.

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