Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

[*N*′-Benzoyl-*N*,*N*-bis(2-pyridylmethyl-κ*N*)ethylenediamine-κ*N*]-chlorocopper(II) hexafluorophosphate

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Received 5 April 2000
Accepted 11 April 2000

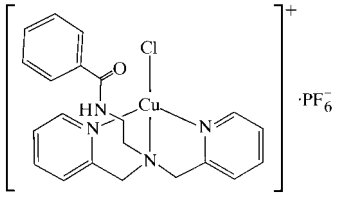
Data validation number: IUC0000107

The title mononuclear copper(II) complex, $[CuCl(C_{21}H_{22}N_4O)]PF_6$, shows a distorted square-planar coordination and the benzoylamino N atom does not coordinate to the Cu atom.

Comment

Crystal structures and catalytic activities of copper(II) complexes containing *N*,*N*′-bis(2-pyridylmethyl)-β-alanineamide ligands were reported by Okuno *et al.* (1997). The copper(II) complexes with similar tripodal ligands containing a peptide group convert supercoiled plasmid DNA into a mixture of nicked and linear forms in the presence of hydrogen peroxide (Kobayashi *et al.*, 1998).

In the crystals of the title compound, $[Cu(dpab)Cl]PF_6$ [(I), dpab is *N*′-benzoyl-*N*,*N*-bis(2-pyridylmethyl)ethylenediamine], the benzoylamino N4 atom does not coordinate to the Cu atom; Cu···N4 = 2.827 (4) Å. The N4—H1 moiety is incorporated in a weak bifurcated hydrogen bond with the F4 and F5 atoms of PF_6; the N4···F4 and N4···F5 distances are 3.421 (9) and 3.383 (10) Å, respectively.



(I)

Experimental

The ligand and its chlorocopper(II) complex were prepared as described previously (Okuno *et al.*, 1997; Kobayashi *et al.*, 1998). Crystals of the title compound were grown from an aqueous methanol/acetonitrile solution.

Crystal data

$[CuCl(C_{21}H_{22}N_4O)]PF_6$	D_x = 1.631 Mg m^{-3}
M_r = 590.4	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 25 reflections
a = 13.064 (3) Å	θ = 10–15°
b = 13.347 (4) Å	μ = 1.155 mm^{-1}
c = 14.077 (3) Å	T = 296 K
β = 101.52 (2)°	Plate, blue
V = 2405.0 (10) Å^3	0.6 × 0.5 × 0.1 mm
Z = 4	

Data collection

Rigaku AFC-5*S* diffractometer	R_{int} = 0.012
θ–2θ scans	θ_{max} = 27.5°
Absorption correction: by integration (Coppens *et al.*, 1965)	$h = 0 \rightarrow 17$
T_{min} = 0.868, T_{max} = 0.966	$k = 0 \rightarrow 17$
5998 measured reflections	$l = -18 \rightarrow 18$
5513 independent reflections	3 standard reflections every 100 reflections
4029 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	H-atom parameters not refined
$R(F)$ = 0.065	$w = 1/[\sigma^2(F_o^2) + \{0.1(F_o^2 + 2F_c^2)/3\}^2]$
$wR(F^2)$ = 0.196	$(\Delta/\sigma)_{max}$ = 0.004
S = 1.38	$\Delta\rho_{max}$ = 0.67 e Å^{-3}
5513 reflections	$\Delta\rho_{min}$ = −0.84 e Å^{-3}
316 parameters	

Table 1
Selected geometric parameters (Å).

Cu1—Cl1	2.249 (1)	Cu1—N2	2.048 (3)
Cu1—N1	1.986 (3)	Cu1—N3	1.991 (4)

Positional parameters of all the H atoms were calculated geometrically and fixed with $U(H) = 1.2U_{eq}$(parent atom).

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

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