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Crystal structure of bis(7-nitro-8-quinolinolato)copper(II), CuC18H10O6N4 / M. Shoja, H. Gershon and D. D. Clarke Fordham University, Department of Chemistry, Fordham Road, Bronx, NY 10458, USA

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Crystal structure of bis(7-nitro-8-quinolinolato)copper(II), $CuC_{18}H_{10}O_6N_4$

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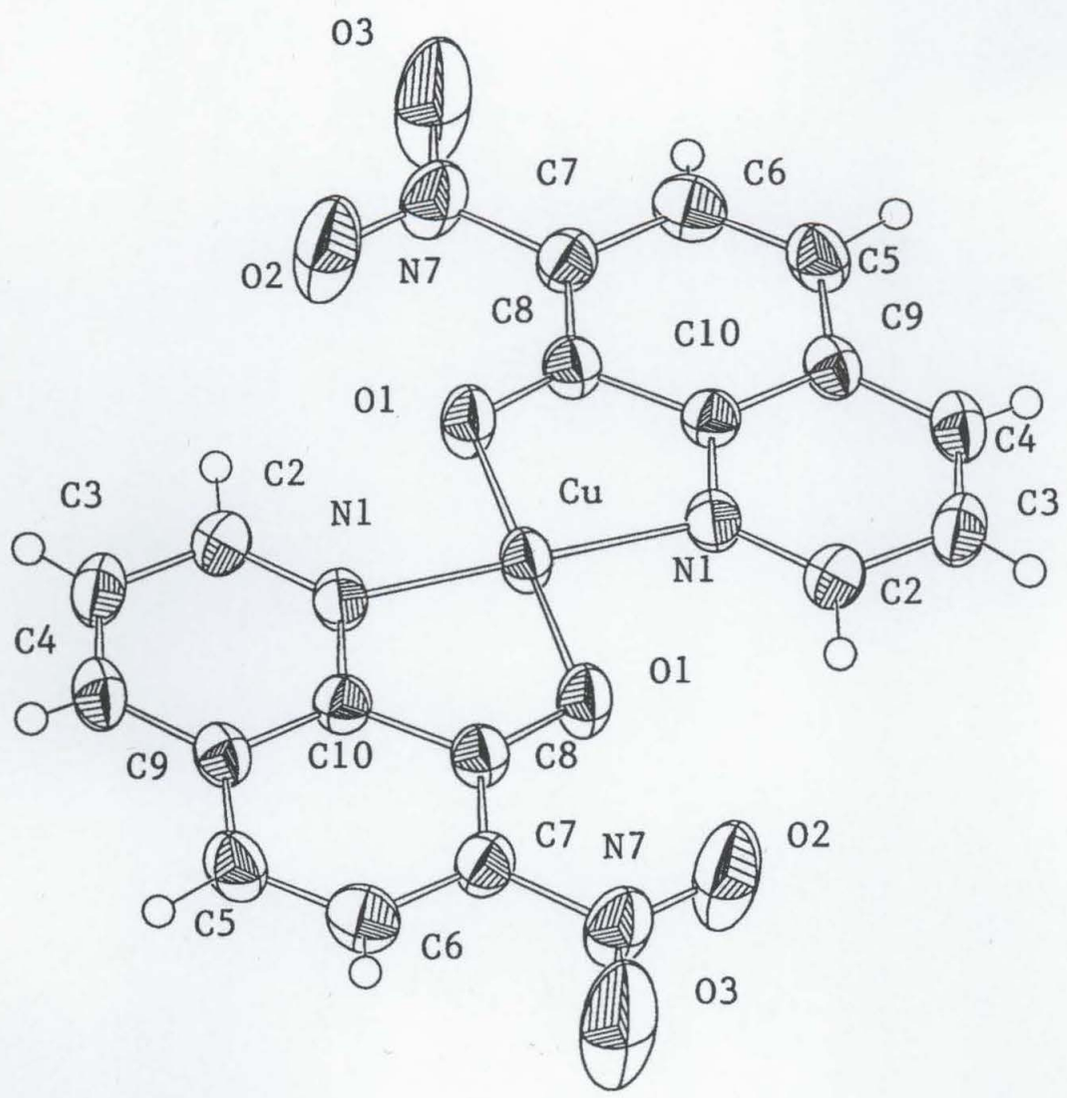

Abstract

$C_{18}H_{10}CuN_4O_6$, monoclinic, $P12_1/c1$ (No. 14), $a = 4.567(9)$ Å, $b = 10.723(8)$ Å, $c = 17.095(6)$ Å, $\beta = 100.0(1)°$, $V = 824.5$ Å^3, $Z = 2$, $R_{gt}(F) = 0.043$, $wR_{gt}(F) = 0.067$, $T = 293$ K.

Source of material

The complex was prepared from the corresponding ligand [1] by standard methods [2]. Crystals grown from dimethyl sulfoxide, mp 625 K – 630 K.

Discussion

The ligands are in square planar arrangement with Cu at the center of symmetry. The Cu—O1 and Cu—N1 bond distances are 1.915(5) Å and 1.962(5) Å, respectedly. We have recently shown that bis(2-methyl-7-nitro-8-quinolinolato) copper(II) and bis(2-methyl-8-quinolinolato)copper(II) are distorted from square planar symmetry [3]. It was of interest therefore to see whether this distortion was due solely to 2-methyl substitution or was also possible in the title compound. The square planar arrangement of the ligands in the title compound was previously predicted based on its inability to inhibit a variety of fungi which were inhibited by the presumably larger molecule bis(2-methyl-7-nitro-8-quinolinolato)copper(II) [3].

Table 1. Data collection and handling.

Crystal:	red prism, size 0.3 × 0.4 × 0.5 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	13.4 cm^{-1}
Diffractometer, scan mode:	Enraf-Nonius CAD4, ω/2θ
$2\theta_{max}$:	50.08°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1641, 1450
Criterion for F_{obs}, $N(hkl)_{gt}$:	$F_{obs} > 3\ \sigma(F_{obs})$, 1260
$N(param)_{refined}$:	153
Program:	Xtal3.4 [4]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2)	4*e*	1.19(1)	1.085(6)	0.680(4)	0.05(2)
H(3)	4*e*	1.07(2)	1.009(7)	0.789(4)	0.06(2)
H(4)	4*e*	0.73(2)	0.854(6)	0.785(4)	0.04(2)
H(5)	4*e*	0.34(2)	0.681(7)	0.712(4)	0.07(2)
H(6)	4*e*	0.21(2)	0.626(8)	0.593(5)	0.06(3)

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu	2*b*	0	0	1/2	0.0406(6)	0.0437(6)	0.0267(5)	–0.0113(5)	0.0048(4)	0.0026(5)
C(2)	4*e*	1.045(1)	1.0150(6)	0.6765(4)	0.045(3)	0.042(4)	0.037(3)	–0.003(3)	0.001(3)	–0.004(3)
N(1)	4*e*	0.924(1)	0.9638(5)	0.6072(3)	0.041(3)	0.040(3)	0.029(3)	–0.002(2)	0.005(2)	0.001(2)
C(10)	4*e*	0.724(1)	0.8697(6)	0.6057(3)	0.034(3)	0.035(3)	0.033(3)	–0.001(3)	0.006(2)	0.000(3)
O(1)	4*e*	0.711(1)	0.8730(4)	0.4663(2)	0.052(3)	0.055(3)	0.029(2)	–0.022(2)	0.008(2)	–0.002(2)
C(8)	4*e*	0.615(1)	0.8231(6)	0.5264(4)	0.038(3)	0.041(3)	0.033(3)	–0.003(3)	0.006(3)	0.001(3)
C(9)	4*e*	0.641(1)	0.8232(6)	0.6752(4)	0.037(3)	0.042(4)	0.033(3)	0.004(3)	0.009(3)	0.005(3)
C(7)	4*e*	0.409(2)	0.7248(6)	0.5234(4)	0.048(4)	0.043(4)	0.036(3)	–0.009(3)	0.009(3)	–0.003(3)
C(3)	4*e*	0.971(2)	0.9721(7)	0.7479(4)	0.050(4)	0.055(5)	0.029(3)	0.004(3)	0.001(3)	–0.005(3)

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Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(4)	4*e*	0.772(2)	0.8781(7)	0.7472(4)	0.049(4)	0.053(4)	0.030(3)	0.002(3)	0.011(3)	0.005(3)
C(5)	4*e*	0.433(2)	0.7222(7)	0.6669(4)	0.050(4)	0.050(4)	0.040(4)	–0.006(3)	0.014(3)	0.008(3)
N(7)	4*e*	0.283(2)	0.6682(6)	0.4467(4)	0.070(4)	0.064(4)	0.046(4)	–0.035(4)	0.013(3)	–0.012(3)
O(2)	4*e*	0.322(2)	0.7147(7)	0.3852(3)	0.108(5)	0.121(6)	0.045(3)	–0.065(4)	0.016(3)	–0.018(4)
C(6)	4*e*	0.325(2)	0.6756(7)	0.5934(5)	0.050(4)	0.048(4)	0.053(5)	–0.016(4)	0.016(4)	0.005(3)
O(3)	4*e*	0.139(3)	0.5791(9)	0.4463(4)	0.30(1)	0.167(8)	0.057(4)	–0.189(9)	0.020(6)	–0.017(5)

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