Crystal structure of bis(2-chloro-6-fluorobenzoato)bis(pyridine)copper(II), $Cu(C_7H_3ClFO_2)_2(C_5NH_5)_2$

F. Valach*[I], A. Saunders[II], A. Cowley[II] and D. J. Watkin[II]

[I] Slovak University of Technology, Faculty of Chemical and Food Technology, Department of Chemical Physics, Radlinského 9, SK-812 37 Bratislava, Slovak Republic

[II] Chemical Crystallography Laboratory, 9 Parks Road, Oxford, OX1 3PD, UK

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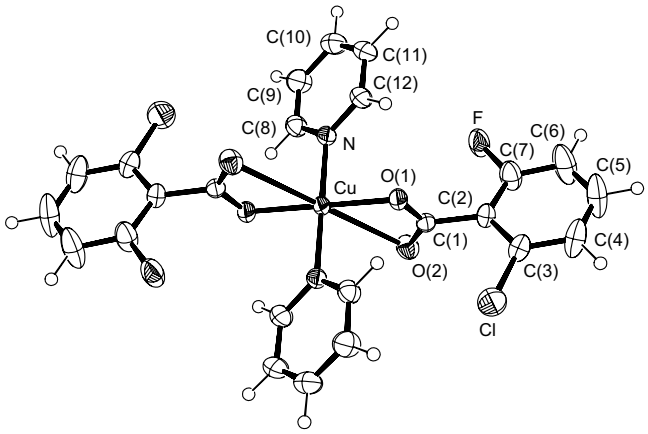

Abstract

$C_{24}H_{16}Cl_2CuF_2N_2O_4$, monoclinic, $P12_1/n1$ (No. 14), $a = 7.119(2)$ Å, $b = 20.845(6)$ Å, $c = 8.316(2)$ Å, $\beta = 104.51(2)°$, $V = 1194.7$ Å^3, $Z = 2$, $R_{gt}(F) = 0.040$, $wR_{obs}(F) = 0.046$, $T = 190$ K.

Source of material

Title compound was prepared according to [1].

Discussion

The title structure consists of centrosymmetric complex units. The bond distances and angles do not show any large deviations. The benzoate O(1)–Cu–O(2) angle (52.55(6)°) is greater than the same angle (43(1)°) in the structure of complex with nicotinamide [2]. But Cu—O(2) bond length (2.780(2) Å) of present structure is shorter than the same internuclear contact (3.141(3) Å) in the complex with nicotinamide.

Table 1. Data collection and handling.

Crystal:	purple block, size 0.70 × 0.70 × 0.70 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	11.88 cm^{-1}
Diffractometer, scan mode:	Enraf-Nonius DIP2000, ω
$2\theta_{max}$:	52.7°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4303, 2444
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 3\ \sigma(I_{obs})$, 2056
$N(param)_{refined}$:	160
Programs:	SIR92 [3], CRYSTALS [4], ORTEP-III [5]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(4)	4*e*	0.6423	–0.0301	1.1110	0.060
H(7)	4*e*	1.141	–0.1026	1.5645	0.050
H(8)	4*e*	1.2125	–0.0547	1.3281	0.060
H(1)	4*e*	1.7984	–0.1850	0.9177	0.063
H(6)	4*e*	0.8085	–0.1154	1.5740	0.051
H(2)	4*e*	1.8008	–0.2645	1.1269	0.071
H(5)	4*e*	0.5557	–0.0766	1.3445	0.049
H(3)	4*e*	1.5392	–0.2737	1.2545	0.073

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*a*	0	0	0	0.0232(2)	0.0250(2)	0.0220(2)	0.0054(1)	0.0027(1)	–0.0005(1)
Cl	4*e*	1.5260(1)	–0.09284(4)	0.7788(1)	0.0526(4)	0.0642(5)	0.0550(4)	0.0067(3)	0.0246(3)	0.0115(3)
O(1)	4*e*	1.2373(2)	–0.05182(7)	1.0448(2)	0.0272(7)	0.0289(7)	0.0281(7)	0.0065(6)	0.0042(6)	–0.0009(6)
O(2)	4*e*	1.0523(2)	–0.11823(8)	0.8628(2)	0.0298(8)	0.0375(8)	0.0377(9)	–0.0003(7)	0.0011(7)	–0.0009(7)
F	4*e*	1.2237(3)	–0.20413(9)	1.1989(2)	0.056(1)	0.066(1)	0.064(1)	0.0316(8)	0.0376(9)	0.0384(9)
N	4*e*	0.9329(3)	–0.03916(9)	1.2001(2)	0.0285(9)	0.0288(9)	0.0237(8)	0.0041(7)	0.0022(7)	–0.0024(7)
C(1)	4*e*	1.2044(3)	–0.1042(1)	0.9623(2)	0.026(1)	0.026(1)	0.0249(9)	0.0020(8)	0.0100(8)	0.0030(8)
C(2)	4*e*	1.3729(3)	–0.1508(1)	1.0011(3)	0.029(1)	0.024(1)	0.038(1)	0.0032(8)	0.0103(9)	–0.0007(8)
C(8)	4*e*	0.7479(3)	–0.0458(1)	1.2084(3)	0.030(1)	0.035(1)	0.032(1)	0.0011(9)	0.0031(9)	–0.0002(9)
C(11)	4*e*	1.0314(4)	–0.0875(2)	1.4690(3)	0.045(2)	0.060(2)	0.026(1)	0.014(1)	0.004(1)	0.007(1)
C(12)	4*e*	1.0723(4)	–0.0599(1)	1.3313(3)	0.032(1)	0.051(1)	0.029(1)	0.010(1)	0.0034(9)	0.004(1)
C(7)	4*e*	1.3827(4)	–0.1979(1)	1.1181(4)	0.041(1)	0.036(1)	0.062(2)	0.007(1)	0.018(1)	0.016(1)

* Correspondence author (e-mail: valach@chelin.chtf.stuba.sk)

Table 3. Continued.

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(4)	4*e*	1.6857(4)	–0.1890(2)	0.9727(5)	0.038(1)	0.047(2)	0.097(3)	0.009(1)	0.029(2)	–0.009(2)
C(3)	4*e*	1.5270(4)	–0.1482(1)	0.9268(3)	0.032(1)	0.033(1)	0.048(1)	0.0006(9)	0.016(1)	–0.006(1)
C(10)	4*e*	0.8416(4)	–0.0945(1)	1.4751(3)	0.051(2)	0.055(2)	0.032(1)	0.003(1)	0.014(1)	0.006(1)
C(5)	4*e*	1.6879(5)	–0.2344(2)	1.0929(6)	0.046(2)	0.041(2)	0.125(3)	0.020(1)	0.020(2)	0.014(2)
C(9)	4*e*	0.6972(4)	–0.0728(1)	1.3429(3)	0.034(1)	0.053(2)	0.041(1)	–0.002(1)	0.010(1)	0.003(1)
C(6)	4*e*	1.5367(5)	–0.2399(2)	1.1677(6)	0.056(2)	0.040(2)	0.109(3)	0.015(1)	0.018(2)	0.032(2)

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