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Structure of the Copper(II) Complex of Isonicotinic Acid

NOBUO OKABE, TOMOKO NAKAMURA AND HATSUKO FUKUDA

Department of Pharmaceutical Sciences, Kinki University, Kowakae, 3-4-1, Higashi Osaka, Osaka 577, Japan

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Abstract

In crystals of diaquabis(isonicotinato-*N*)copper(II) dihydrate, the Cu atom is four-coordinate with the two N atoms of the pyridine rings and the two O atoms of the two water molecules in a *trans* orientation. The coordination geometry is square planar with distances Cu—O 1.985 (2) and Cu—N 2.004 (2) Å.

Comment

Both isoniazid and iproniazid are well known isonicotinic acid derivatives which are used as antituberculosis drugs (Carrington, Bird & Levence, 1984; Pinelopi, 1988), and have bacterial mutagenecity (Parodi *et al.*, 1981). These derivatives inhibit copper(II)-containing serum amine oxidase (Morpurgo *et al.*, 1988; Masuda, Nakamura & Shimomura, 1990). In order to obtain structural information on the mode of interaction between copper(II)-containing amine oxidase and isoniazid and/or iproniazid, we thought it worthwhile to investigate the crystal structure of the complex of isonicotinic acid with copper(II). To date, the crystal structures of the complexes of isonicotinic acid with calcium(II) (Cole & Holt, 1989) and with copper(I) chloride (Goher & Mak, 1985) have been determined, but the complex with copper(II) has not been subjected to crystal-structure analysis.

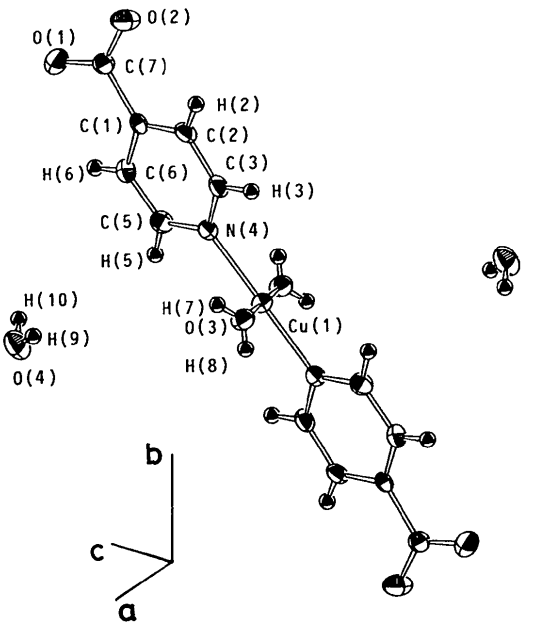

Fig. 1. Perspective view of diaquabis(isonicotinato)copper(II) dihydrate with atomic numbering, along the *a* and *c* axes.

Experimental

Crystal data

$[Cu(C_6H_4NO_2)_2(H_2O)_2].2H_2O$
M_r = 379.81
Triclinic
$P\bar{1}$
a = 6.895 (1) Å
b = 9.181 (1) Å
c = 6.3377 (8) Å
α = 105.24 (1)°
β = 108.20 (1)°
γ = 99.45 (1)°
V = 354.2 (1) Å^3
Z = 1
D_x = 1.781 Mg m^{-3}
D_m = 1.780 (1) Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 25 reflections
θ = 43.5–48.3°
μ = 1.588 mm^{-1}
T = 296 K
Plate
0.40 × 0.40 × 0.30 mm
Blue
Crystal source: solution of isonicotinic acid–$CuCl_2$ (1:7) in 10% ethanol

Data collection

Rigaku AFC-5*R* diffractometer
ω–2θ scans
Absorption correction: *DIFABS* (Walker & Stuart, 1983)
T_{min} = 0.79, T_{max} = 1.29
1756 measured reflections
1621 independent reflections
1487 observed reflections [$I > 3\sigma(I)$]

R_{int} = 0.013
θ_{max} = 55.0°
$h = 0 \rightarrow 8$
$k = -11 \rightarrow 11$
$l = -8 \rightarrow 7$
3 standard reflections monitored every 150 reflections
intensity variation: none

Refinement

Refinement on F^2	$w = 4F_o^2/\sigma^2(F_o^2)$
Final $R = 0.033$	$(\Delta/\sigma)_{max} = 0.05$
$wR = 0.041$	$\Delta\rho_{max} = 0.60$ e Å^{-3}
$S = 1.68$	$\Delta\rho_{min} = -0.69$ e Å^{-3}
1487 reflections	Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)
138 parameters	
All H-atom parameters refined	

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
Cu(1)	0.0	0.0	0.0	1.68 (1)
O(1)	0.4383 (3)	0.7143 (2)	0.9298 (3)	2.86 (6)
O(2)	0.2980 (4)	0.7944 (2)	0.6267 (3)	2.87 (6)
O(3)	0.2043 (3)	0.0413 (2)	−0.1530 (3)	2.04 (5)
O(4)	0.7320 (4)	0.0943 (3)	0.7552 (4)	3.21 (7)
N(4)	0.1253 (3)	0.2183 (2)	0.2323 (3)	1.67 (5)
C(1)	0.2719 (4)	0.5246 (3)	0.5465 (4)	1.59 (6)
C(2)	0.1974 (4)	0.4940 (3)	0.3050 (4)	1.91 (7)
C(3)	0.1277 (4)	0.3412 (3)	0.1545 (4)	1.92 (7)
C(5)	0.2012 (4)	0.2483 (3)	0.4664 (4)	2.10 (7)
C(6)	0.2769 (4)	0.3980 (3)	0.6266 (4)	1.96 (7)
C(7)	0.3431 (4)	0.6915 (3)	0.7157 (4)	1.94 (7)

Table 2. *Geometric parameters* (Å, °)

Cu(1)—O(3)	1.985 (2)	C(1)—C(2)	1.386 (3)
Cu(1)—N(4)	2.004 (2)	C(1)—C(6)	1.386 (3)
O(1)—C(7)	1.251 (3)	C(1)—C(7)	1.516 (3)
O(2)—C(7)	1.255 (3)	C(2)—C(3)	1.377 (3)
N(4)—C(3)	1.345 (3)	C(5)—C(6)	1.376 (3)
N(4)—C(5)	1.343 (3)		
O(3)—Cu(1)—O(3)	180.00	C(6)—C(1)—C(7)	121.6 (2)
O(3)—Cu(1)—N(4)	89.87 (8)	C(1)—C(2)—C(3)	119.6 (2)
N(4)—Cu(1)—N(4)	180.00	N(4)—C(3)—C(2)	122.5 (2)
Cu(1)—N(4)—C(3)	119.6 (2)	N(4)—C(5)—C(6)	122.7 (2)
Cu(1)—N(4)—C(5)	122.6 (2)	C(1)—C(6)—C(5)	119.5 (2)
C(3)—N(4)—C(5)	117.8 (2)	O(1)—C(7)—O(2)	125.9 (2)
C(2)—C(1)—C(6)	117.8 (2)	O(1)—C(7)—C(1)	117.7 (2)
C(2)—C(1)—C(7)	120.6 (2)	O(2)—C(7)—C(1)	116.4 (2)

Data collection, cell refinement: *Rigaku MSC/AFC Data Collection and Refinement Software* (Rigaku Corporation, 1988). The scan rate was 32° min^{-1} in ω and the scan width was (1.68 + 0.30tanθ)°. The ratio of peak counting time to background counting time was 2:1. Programs used to solve structure: *MULTAN*87 (Debaerdemaeker, Germain, Main, Tate & Woolfson, 1987) and *DIRDIF* (Beuskens, 1984). All calculations including data reduction: *TEXSAN* (Molecular Structure Corporation, 1985). Refinement was by full-matrix least squares.

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, complete geometry, bond distances and angles involving H atoms, and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71216 (18 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: OH1018]

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Structure of [Ru(η^6-C_7H_8)(acetylacetonato)Cl]

JAMES G. TOERIEN† AND JAN L. M. DILLEN

Department of Chemistry, University of Pretoria, Pretoria 0002, South Africa

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Abstract

The structure of (acetylacetonato-*O*,*O*′)chloro(η^6-cyclohepta-1,3,5-triene)ruthenium(II), [Ru(η^6-C_7H_8)-{HC(COMe)$_2$}Cl], was determined. The Ru atom lies on a crystallographic mirror plane which is coincident with the molecular mirror plane. The geometry at the Ru atom is, as expected for ruthenium(II), approximately octahedral, with O—Ru—Cl and O—Ru—O bond angles of 84.1 (1) and 90.4 (1)°, respectively.

† Present address: Department of Chemistry and Biochemistry, Rand Afrikaans University, PO Box 524, Johannesburg 2000, South Africa.