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Crystal structure of bis(*N*-(1-(pyrazin-2-yl)ethylidene)nicotinohydrazonato- $\kappa^3 N, N', O$) copper(II) $C_{24}H_{20}N_{10}O_2Cu$

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Abstract

$C_{24}H_{20}N_{10}O_2Cu$, orthorhombic, *Aba2* (no. 41), $a = 12.2281(16)$ Å, $b = 19.176(3)$ Å, $c = 9.8689(13)$ Å, $V = 2314.1(5)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0381$, $wR_{ref}(F^2) = 0.0752$, $T = 296(3)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

All chemicals were purchased except for (*E*)-*N'*-(1-(pyrazin-2-yl)ethylidene)nicotinohydrazide (HL), which was synthesized according to the literature [3]. A mixture of HL (0.05 mmol, 12.1 mg) and $CuSO_4 \cdot 5H_2O$ (0.10 mmol, 25.0 mg) dissolved in ethanol (3 mL) and H_2O (3 mL) was placed in a glass bottle

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	$0.3 \times 0.2 \times 0.2$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.99 mm ⁻¹
Diffractometer, scan mode:	Bruker SMART APEX, ω -scans
θ_{max} , completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	5589, 2028, 0.054
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1424
$N(param)_{refined}$:	186
Programs:	Bruker programs [1], SHELX [2]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U_{iso}^*/U_{eq}
Cu1	1.0000	0.0000	-0.01737(11)	0.0318(3)
O1	0.9965(4)	0.0831(2)	0.1202(4)	0.0458(11)
C1	0.9575(6)	-0.1083(4)	-0.2593(7)	0.0512(19)
H1	1.0325	-0.1166	-0.2584	0.061*
C2	0.8940(6)	-0.1446(4)	-0.3499(8)	0.054(2)
H2	0.9268	-0.1771	-0.4067	0.065*
C3	0.7448(8)	-0.0881(3)	-0.2721(9)	0.0461(16)
H3	0.6700	-0.0795	-0.2741	0.055*
C4	0.8083(5)	-0.0519(3)	-0.1781(7)	0.0347(15)
C5	0.7639(4)	-0.0006(4)	-0.0800(5)	0.0370(14)
C6	0.6436(4)	0.0109(4)	-0.0648(6)	0.047(2)
H6A	0.6310	0.0539	-0.0175	0.071*
H6B	0.6123	-0.0270	-0.0143	0.071*
H6C	0.6103	0.0131	-0.1528	0.071*
C7	0.9005(5)	0.1052(4)	0.1398(7)	0.0376(16)
C8	0.8843(5)	0.1612(4)	0.2430(7)	0.0386(18)
C9	0.9740(6)	0.1917(4)	0.3036(7)	0.057(2)
H9	1.0428	0.1782	0.2732	0.068*
N5	0.9694(5)	0.2388(3)	0.4019(6)	0.065(2)
C11	0.8701(7)	0.2584(4)	0.4418(8)	0.067(2)
H11	0.8646	0.2915	0.5104	0.080*
C12	0.7772(7)	0.2329(4)	0.3879(8)	0.062(2)
H12	0.7097	0.2482	0.4195	0.075*
N1	0.9173(4)	-0.0626(3)	-0.1741(6)	0.0389(14)
N2	0.7853(5)	-0.1340(3)	-0.3584(6)	0.0555(17)
N3	0.8383(3)	0.0312(2)	-0.0119(7)	0.0345(11)
N4	0.8093(4)	0.0811(3)	0.0819(5)	0.0388(14)
C10	0.7827(6)	0.1836(4)	0.2847(7)	0.056(2)
H10	0.7194	0.1663	0.2449	0.067*

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(10 mL) at room temperature. Pale yellow block crystals suitable for single-crystal X-ray diffraction were obtained after 3 days.

Experimental details

The structure was solved by direct methods and refined with the SHELX crystallographic software package [2]. The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Discussion

Hydrazones are well known for their antimicrobial activity and they are subject to current research [4, 5]. But as hydrazones are prone to undergo degradation and bacteria can develop resistance to them, complexation of hydrazones with biocompatible metal ions is useful in this regard for long-term effectiveness [6]. In the course of our studies on the chemistry of lanthanide compounds, we have prepared and characterized a number of complexes containing hydrazones as ligands. Herein we report new Cu(II) complexes derived from (*E*)-*N'*-(1-(pyrazin-2-yl)ethylidene)nicotinohydrazide (HL), producing complexes of the type [Cu(L)₂]. The title complex is a mononuclear coordination compound in which the six coordinated Cu²⁺ is surrounded by two crystallographically dependent acylhydrazones giving a distorted octahedral geometry. The bond lengths of Cu—O and Cu—N (2.066(3)–2.204(4) Å) in the title complex are comparable

with those found in our previous work [7] and there is a structurally related manganese complex [8].

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