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Crystal structure of *N*-(amino(pyrazin-2-yl)methylene)-6-methylpyridin-1-ium-3-carbohydrazonate- $\kappa^3 O, N, N'$ -(dinitrato- $\kappa^1 O$)zinc(II), $C_{12}H_{12}N_8O_7Zn$

Table 1: Data collection and handling.

Crystal:	Yellow rod
Size:	0.24 × 0.06 × 0.04 mm
Wavelength:	Cu K α radiation (1.54178 Å)
μ :	2.75 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	79.7°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	23387, 3416, 0.030
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3271
$N(\text{param})_{\text{refined}}$:	254
Programs:	SHELX [1], Bruker [2]

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Abstract

$C_{12}H_{12}N_8O_7Zn$, monoclinic, $P2_1/c$ (no. 14), $a = 8.2116(3)$ Å, $b = 11.1926(4)$ Å, $c = 17.3488(7)$ Å, $\beta = 96.2450(10)^\circ$, $V = 1585.05(10)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0263$, $wR_{\text{ref}}(F^2) = 0.0722$, $T = 150(2)$ K.

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The molecular structure of the title complex is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The hydrazone ligand, used in this study was prepared according to the literature method while using 6-methylnicotinic acid hydrazide instead of nicotinic acid hydrazide [3]. The crystals of the title complex suitable for the X-ray analysis were obtained by slow evaporation of the ethanol solution of the hydrazone ligand with zinc nitrate.

Experimental details

The structure was solved by direct methods and refined with the SHELX software package [1]. The hydrogen atoms were placed at calculated positions and refined as riding atoms.

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.44852(2)	0.17713(2)	0.32758(2)	0.01909(8)
O1	0.32777(15)	0.32880(10)	0.36491(6)	0.0219(2)
O2	0.29118(15)	0.09741(12)	0.24861(7)	0.0269(3)
O3	0.14928(16)	0.07285(11)	0.34672(7)	0.0285(3)
O4	0.03960(18)	0.03693(16)	0.22983(9)	0.0439(4)
O5	0.61312(16)	0.28718(12)	0.28486(7)	0.0298(3)
O6	0.6016(2)	0.17558(16)	0.18288(9)	0.0461(4)
O7	0.79866(19)	0.30241(16)	0.20616(9)	0.0453(4)
N1	0.63308(17)	0.02162(12)	0.35115(8)	0.0204(3)
N2	0.8661(2)	−0.14766(14)	0.40783(10)	0.0306(3)
N3	0.67811(18)	0.11906(13)	0.55206(8)	0.0242(3)
H3A	0.6408	0.1768	0.5798	0.029*
H3B	0.7521	0.0690	0.5737	0.029*
N4	0.51369(17)	0.17787(11)	0.44165(8)	0.0185(3)
N5	0.45611(16)	0.26981(12)	0.48502(7)	0.0184(3)
N6	0.23729(17)	0.54546(13)	0.59109(8)	0.0217(3)
H6	0.2518	0.5510	0.6420	0.026*
N7	0.15462(17)	0.06803(13)	0.27606(8)	0.0235(3)
N8	0.67324(18)	0.25361(14)	0.22309(8)	0.0278(3)
C1	0.6964(2)	−0.05515(15)	0.30427(10)	0.0247(3)
H1	0.6603	−0.0537	0.2504	0.030*
C2	0.8155(2)	−0.13812(16)	0.33288(11)	0.0288(4)
H2	0.8616	−0.1894	0.2974	0.035*
C3	0.8006(2)	−0.07065(15)	0.45506(10)	0.0256(3)
H3	0.8329	−0.0750	0.5093	0.031*
C4	0.68755(19)	0.01493(14)	0.42742(9)	0.0185(3)
C5	0.62236(19)	0.10750(13)	0.47717(9)	0.0177(3)
C6	0.36222(19)	0.34009(13)	0.43842(9)	0.0172(3)
C7	0.28906(18)	0.44268(13)	0.47743(9)	0.0170(3)
C8	0.30917(19)	0.45412(14)	0.55735(9)	0.0201(3)

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H8	0.3734	0.3977	0.5883	0.024*
C9	0.14376(19)	0.62950(14)	0.55108(9)	0.0197(3)
C10	0.12549(19)	0.62166(14)	0.47121(9)	0.0196(3)
H10	0.0633	0.6803	0.4413	0.024*
C11	0.19699(19)	0.52904(14)	0.43443(9)	0.0190(3)
H11	0.1833	0.5242	0.3794	0.023*
C12	0.0640(2)	0.72285(16)	0.59524(11)	0.0269(4)
H12A	0.0093	0.6850	0.6364	0.040*
H12B	−0.0170	0.7661	0.5601	0.040*
H12C	0.1472	0.7789	0.6183	0.040*

Comment

Pyrazine hydrazones have been attracting much attention because of their strong tendency to chelate to transition metal ions, and their complexes exhibited amazing magnetic, photocatalytic and luminescent properties [3–5]. In this work, the zinc(II) complex of a substituted pyridine-pyrazine-hydrazone ligand was synthesized and characterized by X-ray diffraction.

In the title crystal structure, the central zinc(II) ion is surrounded by a neutral hydrazone ligand (occurring in its ylid form; see the figure) with ON₂ donor set, and two O atoms from two monodentate coordinating nitrate ligands. The Zn(II) possesses a distorted tetragonal pyramidal

coordination geometry with the the geometric index τ value of 0.176 [6]. It should be noted that the C–O distance of the hydrazone is 1.2822(19) Å, indicating the enolation of the C=O double bond [3]. Consequently, the terminal pyridine N atom is protonated for charge balance. In the solid, intermolecular N–H···O hydrogen bonds link the complexes into a two-dimensional supermolecular network parallel to the *bc* plane.

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