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Crystal structure of bis[2-(((3-aminopropyl)imino)methyl)-4-nitro-phenolato- $\kappa^3 N, N', O$]nickel(II), $C_{20}H_{24}N_6NiO_6$

Table 1: Data collection and handling.

Crystal:	Clear light green block
Size:	0.22 × 0.19 × 0.16 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.97 mm ⁻¹
Diffractometer, scan mode:	Bruker Apex-II CCD, φ and ω
$\theta_{\max}$, completeness:	25.0°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	3509, 1852, 0.019
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1754
$N(\text{param})_{\text{refined}}$:	151
Programs:	Bruker [1], Olex2 [2], SHELX [3]

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Abstract

$C_{20}H_{24}N_6NiO_6$, triclinic, $P\bar{1}$ (no. 2), $a = 5.3944(6)$ Å, $b = 10.1144(12)$ Å, $c = 10.9297(12)$ Å, $\alpha = 65.236(3)^\circ$, $\beta = 81.959(3)^\circ$, $\gamma = 79.882(3)^\circ$, $Z = 1$, $V = 531.61(11)$ Å³, $R_{\text{gt}}(F) = 0.0262$, $wR_{\text{ref}}(F^2) = 0.0649$, $T = 173(2)$ K.

CCDC no.: 1875750

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 solvents and other reagents were of analytical grade. Synthesis of the ligand was prepared by a similar method reported earlier [4]. A methanol solution (3.0 mL) of nickel(II) acetate tetrahydrate (3.72 mg, 0.015 mmol) was added to a dichloromethane solution (2.0 mL) of HL : 2-(((3-aminopropyl)imino)methyl)-4-nitro-phenol (4.40 mg,

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.3389(4)	0.1771(2)	0.54273(18)	0.0206(4)
C2	0.5111(4)	0.2699(2)	0.53549(19)	0.0235(4)
H2	0.547524	0.277142	0.614855	0.028*
C3	0.6259(4)	0.3497(2)	0.41251(19)	0.0240(4)
H3	0.743526	0.411483	0.408278	0.029*
C4	0.5753(3)	0.3435(2)	0.29081(18)	0.0177(4)
C5	0.4050(3)	0.2428(2)	0.30268(18)	0.0175(4)
C6	0.2914(4)	0.1612(2)	0.42911(19)	0.0195(4)
H6	0.180625	0.094181	0.436945	0.023*
C7	0.3736(3)	0.2073(2)	0.18999(18)	0.0178(4)
H7	0.312284	0.117283	0.210417	0.021*
C8	0.4358(3)	0.2244(2)	−0.03380(19)	0.0188(4)
H8A	0.331454	0.290631	−0.109262	0.023*
H8B	0.368184	0.129066	0.009263	0.023*
C9	0.7105(4)	0.2017(2)	−0.08818(19)	0.0195(4)
H9A	0.814677	0.141730	−0.010963	0.023*
H9B	0.719484	0.145651	−0.144655	0.023*
C10	0.8226(3)	0.3438(2)	−0.17157(18)	0.0181(4)
H10A	0.993078	0.320713	−0.210498	0.022*
H10B	0.716016	0.405812	−0.247291	0.022*
N1	0.2185(3)	0.09298(18)	0.67192(16)	0.0234(4)
N2	0.4228(3)	0.28871(17)	0.06554(15)	0.0159(3)
N3	0.8408(3)	0.42723(17)	−0.08960(15)	0.0184(3)
H3A	0.918194	0.507404	−0.143334	0.022*
H3B	0.943674	0.369786	−0.022393	0.022*
Ni1	0.500000	0.500000	0.000000	0.01459(12)
O1	0.0577(3)	0.01700(19)	0.67698(15)	0.0402(4)
O2	0.2793(3)	0.09820(16)	0.77417(13)	0.0284(3)
O3	0.6806(2)	0.42554(14)	0.17693(12)	0.0189(3)

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0.005 mmol) at room temperature. After the mixture was stirred for 2 h the mixture was filtered off. The resulting filtrate was left undisturbed for one week to form block crystals. Yield: 40.5%. Elemental analysis – Anal. Calcd. for C₂₀H₂₄N₆NiO₆: C, 47.74%; H, 4.81%; N, 16.70%. Found: C, 47.95%; H, 4.89%; N, 16.55%.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

Schiff base compounds are considered a versatile class of organic ligands [5–8]. Related metal complexes have been investigated for several decades [9–13]. These complexes have been widely used in many fields, such as: optical and catalytic activities [14, 15], magnetic materials [16] and supramolecular structures [17, 18], and also in the field of bio chemistry on [19, 20].

In the crystal structure of the title complex, the title complex is only built up by the C₂₀H₂₄N₆NiO₆ complexes, in which all bond lengths are in normal ranges. The crystal structure shows the title complex has a symmetric mononuclear structure. The hexacoordinated Ni(II) atom is located in a N₄O₂ coordination environment located on an inversion center provided by two deprotonated L[−], wherein the coordinating atoms include N2, N3, O3 and N2' N3', O3'.

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