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Crystal structure of Bis(acetato- κ^2O,O')-bis[4-(dimethylamino)pyridine- κN]nickel(II), $C_{18}H_{26}N_4NiO_4$

Table 1: Data collection and handling.

Crystal:	Green block
Size:	0.43 × 0.32 × 0.16 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.00 mm ⁻¹
Diffractometer, scan mode:	Enraf-Nonius CAD-4, ω
$\theta_{\max}$, completeness:	25.0°, 98%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	2365, 1738, 0.011
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1688
$N(\text{param})_{\text{refined}}$:	124
Programs:	CAD-4 [1], XCAD4 [2], Olex2 [3]

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Abstract

$C_{18}H_{26}N_4NiO_4$, triclinic, $P\bar{1}$ (no. 2), $a = 7.7547(16)$ Å, $b = 7.8666(16)$ Å, $c = 8.2798(17)$ Å, $\alpha = 90.46(3)^\circ$, $\beta = 96.24(3)^\circ$, $\gamma = 93.25(3)^\circ$, $V = 501.24(18)$ Å³, $Z = 1$, $R_{\text{gt}}(F) = 0.0294$, $wR_{\text{ref}}(F^2) = 0.0873$, $T = 310$ K.

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The molecular structure is shown in the figure. In the figure only the asymmetric unit is labelled. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.5	0.5	0.0	0.04087(17)
O1	0.6752(2)	0.4855(2)	0.2841(2)	0.0661(5)
O2	0.45084(19)	0.33073(18)	0.16609(18)	0.0483(4)
N1	0.3319(2)	0.6523(2)	0.0870(2)	0.0453(4)
N2	−0.0213(3)	0.9730(3)	0.2604(3)	0.0610(5)
C1	0.5444(4)	0.2716(4)	0.4412(3)	0.0675(7)
H1a	0.4494(4)	0.1876(4)	0.4219(3)	0.1013(10)*
H1b	0.6498(4)	0.2162(4)	0.4722(3)	0.1013(10)*
H1c	0.5224(4)	0.3478(4)	0.5269(3)	0.1013(10)*
C2	0.5622(3)	0.3709(3)	0.2885(3)	0.0473(5)
C3	0.1833(3)	0.5919(3)	0.1409(3)	0.0502(5)
H3	0.1607(3)	0.4745(3)	0.1399(3)	0.0602(6)*
C4	0.0632(3)	0.6911(3)	0.1972(3)	0.0519(5)
H4	−0.0381(3)	0.6407(3)	0.2307(3)	0.0623(6)*
C5	0.0920(3)	0.8688(3)	0.2046(3)	0.0466(5)
C6	0.2488(3)	0.9326(3)	0.1500(3)	0.0478(5)
H6	0.2771(3)	1.0491(3)	0.1525(3)	0.0574(6)*
C7	0.3594(3)	0.8220(3)	0.0932(3)	0.0474(5)
H7	0.4608(3)	0.8682(3)	0.0564(3)	0.0568(6)*
C8	0.0066(4)	1.1563(3)	0.2604(4)	0.0678(7)
H8a	−0.0879(4)	1.2074(3)	0.3045(4)	0.1017(10)*
H8b	0.1136(4)	1.1891(3)	0.3255(4)	0.1017(10)*
H8c	0.0128(4)	1.1940(3)	0.1510(4)	0.1017(10)*
C9	−0.1892(4)	0.9084(4)	0.3024(4)	0.0798(8)
H9a	−0.2512(4)	1.0008(4)	0.3395(4)	0.1197(13)*
H9b	−0.2546(4)	0.8553(4)	0.2085(4)	0.1197(13)*
H9c	−0.1731(4)	0.8263(4)	0.3871(4)	0.1197(13)*

Source of material

A mixture of Ni(CH₃CO₂)₂·H₂O (0.2 g, 0.01 mol) and 4-(dimethylamino)pyridine (DMAP) (0.15 g, 1 mmol) were mixed in methanol (40 mL) and stirred in refluxing for 8 h. The reacted mixture was filtered, and the filtrate was allowed to stand for 16 days to finally obtain small green block-like crystals of the title complex.

Experimental details

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

Comment

Metal-organic coordination polymers (CPs) have received extensive attention due to their structural diversity and their potential applications in molecular adsorption, separation, gas storage, ion exchange, catalysis and sensing [4, 5].

The molecular structure of the title compound is shown in the figure. In the title complex, Ni(II) ions located at the center of inversion are coordinated by two N atoms of the two 4-(dimethylamino)pyridine (DMAP) ligands at the top and four O atoms of two crystallographically related acetate anions. In the coordination geometry, the Ni1-N1, Ni1-O1 and Ni1-O2 bond lengths are 2.005, 2.592 and 1.974 Å respectively, in a regular distance range [6–8]. The N1-Ni1-O1, N1-Ni1-O2 and O1-Ni1-O2 bond angles are 88.798(59), 90.563(63) and 55.610(56)°, respectively. Generally all bond lengths in all moieties are in the expected ranges [9].

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