Crystal structure of *bis*-{1-[1-(3-aminopentylimino)ethyl]naphthalen-2-olato}nickel(II), $[Ni(C_{17}H_{21}N_2O)_2]$, $C_{34}H_{42}N_4NiO_2$

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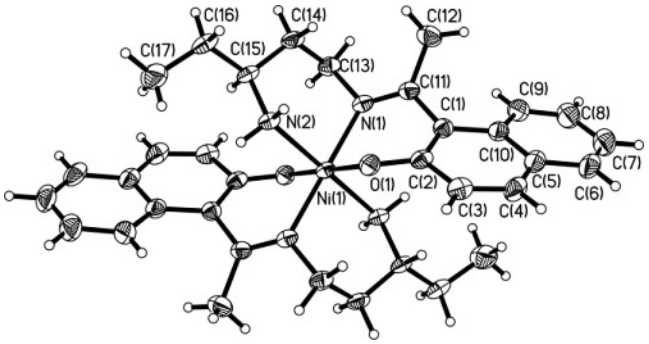

Abstract

$C_{34}H_{42}N_4NiO_2$, monoclinic, $P2_1/n$ (no. 14), a = 9.426(2) Å, b = 15.610(3) Å, c = 10.018(2) Å, β = 92.115(2)°, V = 1473.0 Å^3, Z = 2, $R_{gt}(F)$ = 0.0699, $wR_{ref}(F^2)$ = 0.1333, T = 298 K.

Table 1. Data collection and handling.

Crystal:	green blocks, size 0.26×0.27×0.31 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	6.97 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD area-detector, ω
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	10619, 2744
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1644
$N(param)_{refined}$:	189
Programs:	SHELX [13]

Source of material

1-(2-hydroxynaphthalen-1-yl)ethanone (0.19 g, 1 mmol) and propane-1,3-diamine (0.10 g, 1 mmol) were mixed and stirred in methanol (20 mL) at room temperature for 30 min. Then to the mixture was added with stirring a methanolic solution (10 mL) of nickel acetate (0.25 g, 1 mmol). The final mixture was further stirred at room temperature for 30 min, and filtered. Green, block-shaped single crystals of the complex, suitable for X-ray diffraction were formed during slow evaporation of the solution in air.

Experimental details

Hydrogen atoms were positioned geometrically and constrained to ride on their parent atoms, with C–H distances of 0.93-0.97 Å, N–H distances of 0.90 Å, and with $U_{iso}(H) = 1.2U_{eq}(C,N)$ and $1.5U_{eq}(C_{methyl})$.

Discussion

Schiff base ligands containing strong donor sites like phenoxo oxygen atoms as well as imine nitrogen atoms have received considerable attention for the construction of versatile complexes with transition metal ions [1-4]. The nickel complexes with Schiff base ligands have been proved to have interesting catalytic [5, 6], magnetic [7, 8], and biological activities [9, 10]. In the present paper, the synthesis and structure of a new nickel(II) complex with the Schiff base ligand 1-[1-(3-amino-pentylimino)ethyl] naphthalen-2-ol is reported. The complex is a mono nuclear nickel(II) compound (see Fig.), which possesses a crystallo-graphic inversion symmetry. The Ni atom, lying on the inversion center, is six-coordinated by two phenolate O, two imine N, and two amine N atoms from two Schiff base ligands, forming an octahedral geometry. The Ni–O and Ni–N bond lengths are within normal values as those observed in similar nickel(II) complexes [11, 12]. The six-membered chelate ring Ni(1)–N(1)–C(13)–C(14)–C(15)–N(2) adopts a chair conformation, with the two atoms Ni(1) and C(14) deviate from the least-squares plane defined by the remaining four atoms by 1.007(3) and 0.703(3) Å, respectively.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2A)	4*e*	0.3722	0.0401	0.7085	0.051
H(2B)	4*e*	0.3744	0.1160	0.6263	0.051
H(3)	4*e*	0.8262	0.1974	0.4662	0.063
H(4)	4*e*	0.9320	0.2339	0.2751	0.072
H(6)	4*e*	0.9447	0.2242	0.0281	0.085
H(7)	4*e*	0.8432	0.1840	–0.1736	0.095
H(8)	4*e*	0.6262	0.1168	–0.1830	0.091
H(9)	4*e*	0.5057	0.0912	0.0043	0.072
H(12A)	4*e*	0.2791	0.1125	0.1018	0.096
H(12B)	4*e*	0.3734	0.1949	0.1174	0.096
H(12C)	4*e*	0.2503	0.1786	0.2154	0.096
H(13A)	4*e*	0.2146	–0.0305	0.3655	0.060
H(13B)	4*e*	0.1816	0.0437	0.2634	0.060
H(14A)	4*e*	0.1889	0.1411	0.4493	0.060
H(14B)	4*e*	0.0582	0.0792	0.4442	0.060
H(15)	4*e*	0.1744	–0.0087	0.6041	0.051
H(16A)	4*e*	0.1399	0.1574	0.7067	0.065
H(16B)	4*e*	0.0131	0.0944	0.6781	0.065
H(17A)	4*e*	0.1155	0.0000	0.8406	0.128
H(17B)	4*e*	0.0691	0.0875	0.9020	0.128
H(17C)	4*e*	0.2295	0.0705	0.8753	0.128

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ni(1)	2*c*	½	0	½	0.0262(4)	0.0424(5)	0.0436(5)	0.0005(5)	–0.0008(3)	–0.0025(5)
O(1)	4*e*	0.5990(3)	0.1169(2)	0.4995(3)	0.040(2)	0.048(2)	0.049(2)	–0.005(2)	0.002(2)	–0.001(2)
N(1)	4*e*	0.3806(4)	0.0482(2)	0.3424(4)	0.032(2)	0.045(2)	0.046(3)	0.003(2)	–0.002(2)	–0.008(2)
N(2)	4*e*	0.3537(3)	0.0597(2)	0.6252(4)	0.030(2)	0.047(2)	0.052(3)	0.005(2)	–0.002(2)	–0.002(2)
C(1)	4*e*	0.5755(5)	0.1283(3)	0.2614(5)	0.042(3)	0.037(3)	0.048(3)	0.001(2)	0.001(2)	0.001(2)
C(2)	4*e*	0.6467(5)	0.1415(3)	0.3856(5)	0.038(3)	0.029(3)	0.063(4)	0.004(2)	0.004(3)	–0.005(3)
C(3)	4*e*	0.7810(5)	0.1838(3)	0.3849(5)	0.048(3)	0.035(3)	0.074(4)	–0.003(2)	–0.002(3)	–0.005(3)
C(4)	4*e*	0.8456(5)	0.2051(3)	0.2704(6)	0.046(3)	0.039(3)	0.096(5)	–0.008(2)	0.017(3)	0.004(3)
C(5)	4*e*	0.7831(6)	0.1840(3)	0.1447(6)	0.053(3)	0.036(3)	0.075(4)	0.006(2)	0.019(3)	0.005(3)
C(6)	4*e*	0.8558(6)	0.1981(3)	0.0247(7)	0.062(4)	0.044(3)	0.108(5)	0.012(3)	0.039(4)	0.011(4)
C(7)	4*e*	0.7959(7)	0.1737(4)	–0.0953(7)	0.095(5)	0.075(5)	0.069(5)	0.024(4)	0.040(4)	0.006(4)
C(8)	4*e*	0.6654(7)	0.1339(4)	–0.1007(6)	0.094(5)	0.070(4)	0.065(4)	0.022(4)	0.026(4)	0.002(3)
C(9)	4*e*	0.5928(6)	0.1191(3)	0.0113(5)	0.062(4)	0.064(4)	0.055(4)	0.008(3)	0.007(3)	0.002(3)
C(10)	4*e*	0.6470(5)	0.1455(3)	0.1396(5)	0.048(3)	0.039(3)	0.060(4)	0.009(2)	0.010(3)	0.005(3)
C(11)	4*e*	0.4247(5)	0.1036(3)	0.2583(5)	0.039(3)	0.049(3)	0.042(3)	0.006(2)	–0.004(2)	–0.005(3)
C(12)	4*e*	0.3225(5)	0.1519(3)	0.1646(5)	0.064(4)	0.070(4)	0.057(4)	0.009(3)	–0.011(3)	0.004(3)
C(13)	4*e*	0.2282(4)	0.0301(3)	0.3487(5)	0.033(3)	0.056(3)	0.060(3)	–0.006(2)	–0.008(2)	–0.003(3)
C(14)	4*e*	0.1605(4)	0.0817(3)	0.4580(5)	0.026(3)	0.055(3)	0.069(4)	0.001(2)	–0.005(2)	0.003(3)
C(15)	4*e*	0.1980(4)	0.0523(3)	0.5995(5)	0.025(2)	0.037(3)	0.065(4)	0.004(2)	0.005(2)	–0.007(3)
C(16)	4*e*	0.1131(5)	0.0974(3)	0.7044(5)	0.029(3)	0.052(3)	0.082(4)	0.002(2)	0.006(3)	–0.016(3)
C(17)	4*e*	0.1337(6)	0.0605(4)	0.8432(5)	0.083(4)	0.111(5)	0.063(4)	0.033(4)	0.011(3)	–0.013(4)

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