Instrumental Achievements

Crystal Structure of [1-{(2-Oxyphenyl)iminomethyl}benzen-2-oxy-*N,O,O'*](cyclopropylamine-*N*)nickel(II) Complex

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The structures of monomeric Ni complexes in the presence of a tridentate ONO or ONS Schiff-base ligand and different monodentate ligands (piperidine[1], pyrrolidine[2] and cyclohexylamine[3]) were reported previously. In those complexes the Ni ion has either a square or distorted square-planar coordination. Here, we report on the structure of a new Ni complex, which has as a monodentate ligand the cyclopropylamine molecule (Fig. 1). As can be seen from Fig. 2, the coordination around the Ni ion in the title complex is also distorted square planar. The Ni–O and Ni–N bond lengths are [1.814(5) – 1.866(5)Å] and [1.846(6) – 1.929(5)Å], respectively. The coordination angles around the Ni ion range from 86.5(2) to 96.6(3)°. The Ni ion is 0.0218(9)Å out of the best plane going through the atoms O1, N1, O2, N2. The dihedral angle between the two moieties (O1, C1–C7 and N1, C8–C13, O2) of the tridentate ligand is 6(2)°. The cyclopropyl ring is folded toward the coordination plane due to van der Waals forces. The dihedral angle between the coordination plane (O1, N1, O2, N2) and the C14, C15, C16 ring is 67.3(4)°.

Table 1 shows the crystal and experimental data, while the final atomic parameters are given in Table 2. The bond distances and angles are shown in Table 3. The chemical reaction of the title compound is shown in Fig. 1.

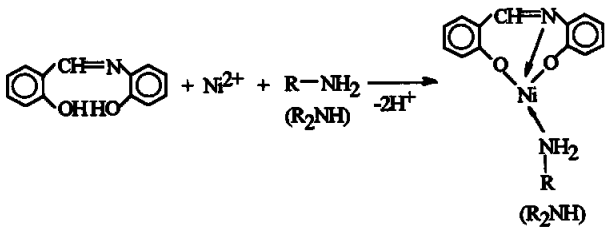

Fig. 1 Synthesis and chemical structure.

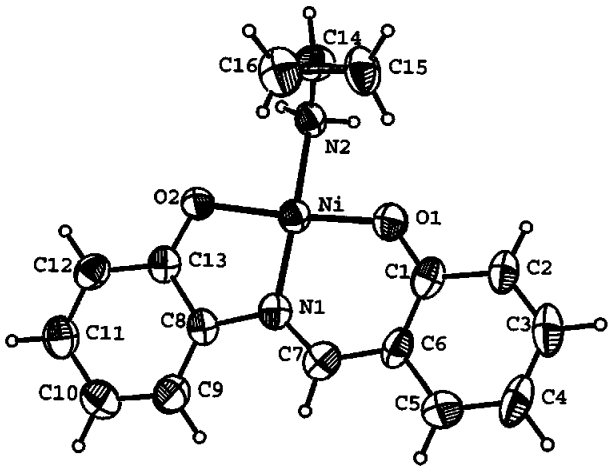

Fig. 2 ORTEP drawing of the title compound with atom labeling.

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Table 1 Crystal and experimental data

Formula:	$C_{16}H_{16}N_2NiO_2$
Formula weight=	327.03
Crystal system:	monoclinic
Space group:	$C2/c$ $Z=8$
a=	30.206(3)Å
b=	4.896(2)Å
c=	20.476(2)Å
β=	112.054(3)°
V=	2806.6(5)Å^3
D_x=	1.548 g/cm^3
μ(Mo K$_\alpha$)=	1.392 mm^{-1}
T=	295 K
Dark red	
F(0 0 0)=	1360
Crystal size:	0.4×0.1×0.08 mm
Radiation=	Mo K$_\alpha$
R=	0.050
Rw=	0.048
No. of reflections used=	1193
No. of parameters=	190
Goodness-of-fit=	1.23
Measurement:	Enraf Nonius CAD-4 diffractometer
Program system:	CAD-4 EXPRESS Software
Structure determination:	MolEN
Treatment of hydrogen atoms:	geometric calculation
Refinement:	full matrix least-squares (MolEN)

Table 2 Final atomic coordinates and equivalent isotropic thermal parameters for non-hydrogen atoms

Atom	x	y	z	B_{eq}/Å^2
Ni	0.59767(3)	0.0531(2)	0.05881(4)	2.86(2)
O1	0.6368(1)	0.317(1)	0.1121(2)	3.6(1)
O2	0.5554(1)	-0.220(1)	0.0091(2)	3.2(1)
N1	0.6391(2)	-0.076(1)	0.0188(2)	3.0(1)
N2	0.5499(2)	0.195(1)	0.0912(3)	3.1(1)
C1	0.6812(2)	0.364(1)	0.1206(3)	3.3(2)
C2	0.7071(2)	0.568(2)	0.1671(3)	3.7(2)
C3	0.7537(3)	0.624(2)	0.1791(4)	4.6(2)
C4	0.7769(2)	0.480(2)	0.1423(3)	4.8(2)
C5	0.7530(2)	0.283(2)	0.0955(4)	4.3(2)
C6	0.7051(2)	0.222(2)	0.0831(4)	3.4(2)
C7	0.6824(2)	0.011(1)	0.0336(3)	3.5(2)
C8	0.6182(2)	-0.285(1)	-0.0311(3)	2.7(2)
C9	0.6370(2)	-0.408(2)	-0.0754(3)	3.7(2)
C10	0.6119(2)	-0.612(2)	-0.1207(3)	4.0(2)
C11	0.5678(2)	-0.692(2)	-0.1209(3)	3.9(2)
C12	0.5484(2)	-0.566(2)	-0.0775(3)	3.4(2)
C13	0.5728(2)	-0.355(1)	-0.0321(3)	2.8(2)
C14	0.5488(2)	0.111(2)	0.1588(3)	3.8(2)
C15	0.5929(3)	0.117(2)	0.2225(4)	4.4(2)
C16	0.5710(3)	-0.147(2)	0.1910(4)	4.9(2)

$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* (\boldsymbol{a}_i \cdot \boldsymbol{a}_j)$.

Table 3 Bond distances (Å) and angles (°)

Ni - O1	1.814(5)	C4 - C5	1.36(1)
Ni - O2	1.866(5)	C5 - C6	1.41(1)
Ni - N1	1.846(6)	C6 - C7	1.43(1)
Ni - N2	1.929(5)	C8 - C9	1.38(1)
O1 - C1	1.308(8)	C8 - C13	1.41(1)
O2 - C13	1.323(8)	C9 - C10	1.38(1)
N1 - C7	1.300(8)	C10 - C11	1.39(1)
N1 - C8	1.413(9)	C11 - C12	1.38(1)
N2 - C14	1.458(9)	C12 - C13	1.40(1)
C1 - C2	1.40(1)	C14 - C15	1.473(9)
C1 - C6	1.42(1)	C14 - C16	1.46(1)
C2 - C3	1.36(1)	C15 - C16	1.48(1)
C3 - C4	1.40(1)		
O1 - Ni - O2	175.7(2)	C1 - C6 - C5	119.7(8)
O1 - Ni - N1	96.6(3)	C1 - C6 - C7	122.2(7)
O1 - Ni - N2	86.5(2)	C5 - C6 - C7	118.1(8)
O2 - Ni - N1	87.1(3)	N1 - C7 - C6	125.2(7)
O2 - Ni - N2	89.9(2)	N1 - C8 - C9	127.6(7)
N1 - Ni - N2	174.3(2)	N1 - C8 - C13	110.7(7)
Ni - O1 - C1	127.5(5)	C9 - C8 - C13	121.7(7)
Ni - O2 - C13	110.5(4)	C8 - C9 - C10	120.1(7)
Ni - N1 - C7	125.1(6)	C9 - C10 - C11	119.5(8)
Ni - N1 - C8	112.1(5)	C10 - C11 - C12	120.5(8)
C7 - N1 - C8	122.8(7)	C11 - C12 - C13	121.0(7)
Ni - N2 - C14	120.8(5)	O2 - C13 - C8	119.2(7)
O1 - C1 - C2	119.9(8)	O2 - C13 - C12	123.7(7)
O1 - C1 - C6	123.2(7)	C8 - C13 - C12	117.1(8)
C2 - C1 - C6	116.9(7)	N2 - C14 - C15	119.9(7)
C1 - C2 - C3	122.8(8)	N2 - C14 - C16	120.1(7)
C2 - C3 - C4	119.6(8)	C15 - C14 - C16	60.7(5)
C3 - C4 - C5	120.0(8)	C14 - C15 - C16	59.3(5)
C4 - C5 - C6	121.1(8)	C14 - C16 - C15	60.0(5)

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