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Bis[2-(4,5-dihydro-1*H*-imidazol-2-yl)phenolato-κ^2N,O]nickel(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.029
wR factor = 0.083
Data-to-parameter ratio = 12.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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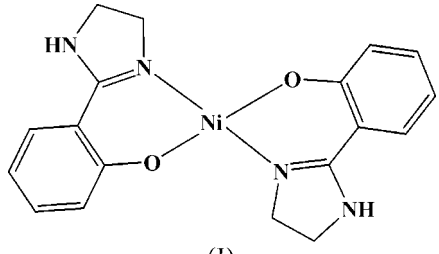
In the title complex, $[Ni(C_9H_9N_2O)_2]$, the Ni^{2+} ion is coordinated by two 2-(4,5-dihydro-1*H*-imidazol-2-yl)phenolate ligands. Each ligand provides one O atom and one N atom to the Ni coordination, giving a total coordination number of 4. The centrosymmetric complex adopts a square-planar geometry.

Comment

The structures of the Cu^{2+}, Zn^{2+} and Ni^{2+} complexes of 2-(1*H*-imidazol-2-yl)phenol have previously been studied by IR spectroscopy (Lane *et al.* 1962). The results indicated that this ligand chelates to metal ions through imidazolyl N and phenolate O atoms. However, no single-crystal structure of these complexes was reported. To shed some light on how this ligand interacts with different metal ions, we prepared its very similar derivative 2-(4,5-dihydro-1*H*-imidazol-2-yl)phenol and studied the effect of different metal ions on the geometry of the resulting complexes. The crystal structure of its Ni^{2+} complex is reported here.



(I)

The title compound, (I), was obtained as air-stable, dark-red crystals. As shown in Fig. 1, the Ni^{2+} ion, on an inversion center, is coordinated by two ligands; each provides one phenolate O atom and one imidazolyl N atom. The total coordination number is four and the geometry can be best described as square planar. The imidazolyl ring and the benzene ring lie almost in the same plane, with an angle of 2.21 (18)° between their least-squares planes (C1/C2/N2/C3/N1 and C4–C9).

Experimental

2-(4,5-Dihydro-1*H*-imidazol-2-yl)phenol (58 mg, 0.37 mmol), which was prepared according to the literature method (Bishop *et al.*, 2002), and nickel(II) perchlorate hexahydrate (65 mg, 0.18 mmol) were dissolved separately in methanol (5 ml). The solutions were mixed and stirred for 0.5 h. The clear solution was then kept at room temperature. Dark-red crystals were obtained after one week. Yield 37 mg, 54%.

Crystal data

$[Ni(C_9H_9N_2O)_2]$
M_r = 381.07
Monoclinic, $P2_1/c$
a = 8.0502 (16) Å
b = 5.5733 (11) Å
c = 17.698 (4) Å
β = 94.88 (3)°
V = 791.1 (3) Å^3
Z = 2
D_x = 1.600 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.25 mm^{-1}
T = 293 (2) K
Prism, red
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1K CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.706, T_{max} = 0.789
7742 measured reflections
1522 independent reflections
1187 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.083
S = 1.04
1522 reflections
119 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.0978P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1^{i}	1.8298 (19)	Ni1—N1	1.8801 (17)
O1^{i}—Ni1—O1	180	O1—Ni1—N1	92.65 (7)
O1^{i}—Ni1—N1	87.35 (7)	N1—Ni1—N1^{i}	180

Symmetry code: (i) $-x+1, -y+1, -z+1$.

The position and U_{iso} parameter were refined for the H atom bound to N2 [refined distance H—N = 0.76 (3) Å], while the other H atoms were geometrically constrained and refined in riding mode as follows: C—H = 0.93 and 0.97 Å, U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

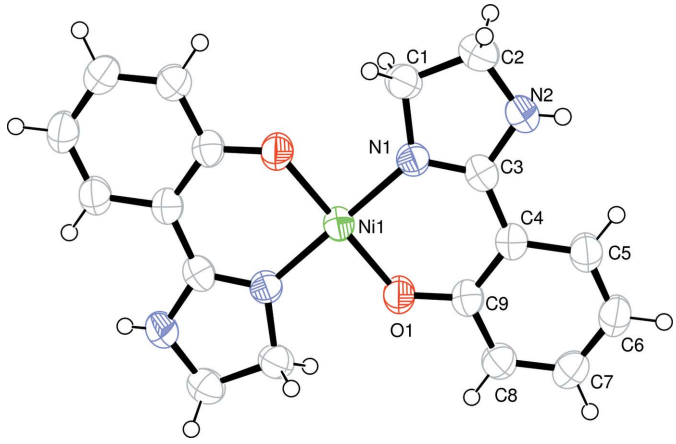


Figure 1
The *ORTEP-3* diagram of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as small circles of arbitrary radii. Unlabeled atoms are related to labeled atoms by the symmetry code $(-x+1, -y+1, -z+1)$.

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