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Bis[(*E*)-*N*′-(2-nitrobenzylidene)-2-oxidobenzohydrazide]bis(pyridine-κ*N*)nickel(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.111
Data-to-parameter ratio = 18.0

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

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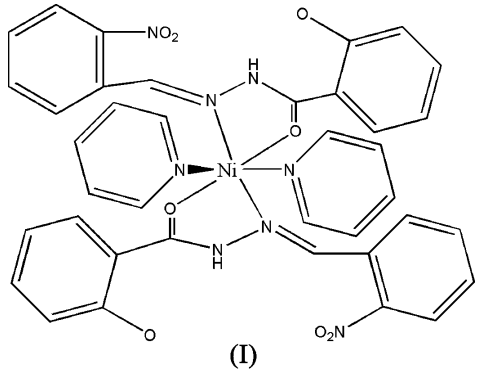
The title compound, $[Ni(C_{14}H_{10}N_3O_4)_2(C_5H_5N)_2]$, contains a Ni atom (site symmetry 2) six-coordinated by two *N*,*O*-bidentate Schiff base ligands and two pyridine N atoms, giving a distorted *trans*-NiN_4O_2 octahedral coordination environment for the metal atom.

Comment

Recently, we have reported some Schiff base complexes (Qiu *et al.*, 2004; Zhu *et al.*, 2003). As an extension of this work the synthesis and structure of the title nickel(II) complex, (I) (Fig. 1), is reported here. The Ni atom (site symmetry 2) in (I) is six-coordinated by two N atoms and two O atoms from two Schiff base ligands and two N atoms from two pyridine molecules. The Schiff base acts as a bidentate ligand and ligates to the Ni atom through an O atom and an N atom. The three *trans* angles at Ni are close to 180°. The *cis* bond angles range from 77.61 (5) to 101.97 (5)°, which indicates a slightly distorted octahedral geometry about Ni.



(I)

The Ni1—O2 bond length in (I) is comparable to the value of 2.038 (2) Å observed by us in a similar nickel(II) compound (You *et al.*, 2004). The Ni—N bond distances are a little longer than the value of 2.068 (3) Å observed in the nickel(II) complex cited above. The conformation of the five-membered chelate ring containing atoms Ni1, O2, C7, N1 and N2 is close to planar.

Experimental

A methanol (10 ml) and pyridine (4 ml) mixture of $Ni(CH_3COO)_2\cdot 6H_2O$ (0.5 mmol, 142.5 mg) was added to a methanol (10 ml) solution of H*L* (1.0 mmol, 285.0 mg), where H*L* is (*E*)-*N*′-(2-nitrobenzylidene)-2-hydroxybenzohydrazide. The reaction mixture was stirred for 20 min to give a green solution. After standing in air for 8 d, green blocks of (I) formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed three times with

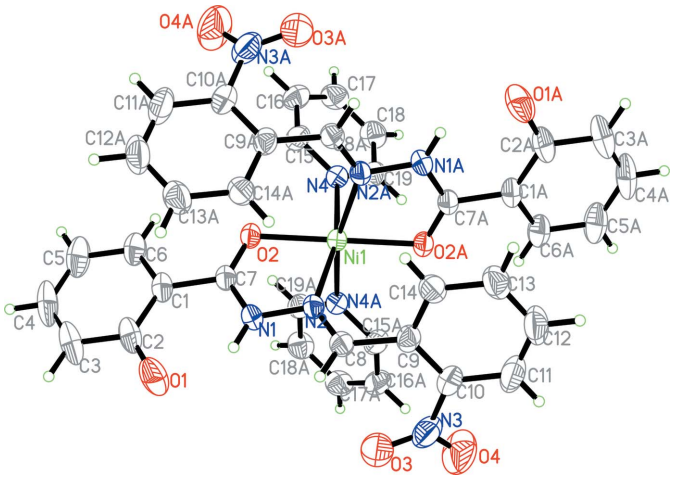


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms). Atoms with the suffix *A* are generated by the symmetry operation $(\frac{3}{2} - x, 2 - y, z)$.

methanol and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 63%).

Crystal data

$[Ni(C_{14}H_{10}N_3O_4)_2(C_5H_5N)_2]$
M_r = 785.41
Orthorhombic, *Ccca*
a = 14.9148 (2) Å
b = 22.1842 (4) Å
c = 22.4259 (4) Å
V = 7420.1 (2) Å^3
Z = 8
D_x = 1.406 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.59 mm^{-1}
T = 298 (2) K
Block, green
0.46 × 0.24 × 0.13 mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.841, T_{max} = 0.925
22385 measured reflections
4484 independent reflections
3308 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 28.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.111
S = 1.02
4484 reflections
249 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2 + 3.9687P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—O2	2.0064 (11)	Ni1—N2	2.1416 (14)
Ni1—N4	2.1184 (15)		

All H atoms were placed in geometrically idealized positions (C—H = 0.93 and N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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