Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[2-Oxido-1-naphthaldehyde (2-hydroxybenzoyl)hydrazonato]pyridinenickel(II)

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Received 9 June 2005
Accepted 13 June 2005
Online 24 June 2005

Key indicators

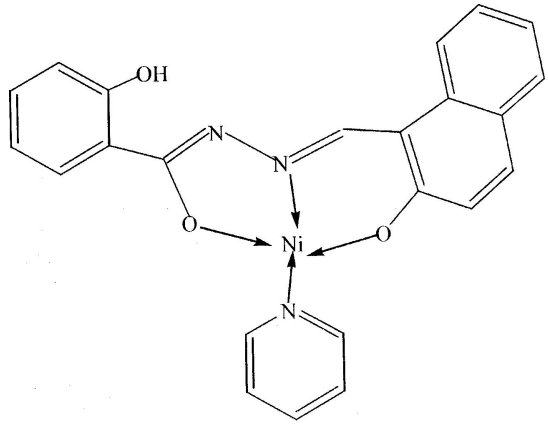
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.092
Data-to-parameter ratio = 12.3

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

The title complex, [Ni($C_{18}H_{12}N_2O_3$)(C_5H_5N)], has a slightly distorted square-planar coordination of the Ni atom with *trans* N atoms [Ni—N = 1.902 (2) and 2.002 (2) Å, Ni—O = 1.880 (2) and 1.927 (2) Å, N—Ni—N = 171.30 (9)° and O—Ni—O = 173.87 (8)°]. The 2-hydroxybenzoyl hydroxy group forms an intramolecular O—H···N hydrogen bond with an adjacent N atom [N···O = 2.591 (3) Å]. Inversion-related molecules have short Ni···N separations of 3.274 (3) and 3.489 (3) Å, and exhibit concomitant π–π stacking; the centroid of the benzoyl ring is some 3.34 Å from the naphthalene plane of the inversion-related molecule.

Comment

A view of the molecule of the title compound, (I), is shown in Fig. 1. Molecular dimensions are normal and are available in the archived CIF.



(I)

There is an intramolecular O2—H2···N2 hydrogen bond (Table 1). Inversion-related pairs of molecules have Ni···N intermolecular separations of Ni1···N2^{i} = 3.274 (3) Å and Ni1···N1^{i} 3.489 (3) Å [symmetry code: (i) $1-x, 2-y, 1-z$]. There are concomitant π–π interactions, the centroid of aromatic ring C2–C7 being some 3.34 Å from the C9–C13 ring of the naphthalene plane at $(1-x, 2-y, 1-z)$.

For related literature, see Adams *et al.* (1998, 2000), Bhatia *et al.* (1983), Blake *et al.* (2000), Burchell *et al.* (2004), Cheng *et al.* (1996), Figueiredo *et al.* (2000), Gan *et al.* (2004), Guo *et al.* (2005), He *et al.* (2002), Hou *et al.* (2005), Janiak (2000), Jiang *et al.* (1998), Ranford *et al.* (1998), Sakamoto *et al.* (1989), Tabbi *et al.* (1999), Wang *et al.* (1998), Wu & Liu (2004), Xiao *et al.* (2004), Xu *et al.* (2001), Yan *et al.* (1993), Yang *et al.* (2003) and Zhang *et al.* (2005).

Experimental

The synthesis of the title complex was carried out by mixing the ligand (0.077 g, 0.25 mmol) in dimethylformamide (5 ml) and $NiCl_2·6H_2O$ (0.058 g, 0.25 mmol) in a mixed methanol–pyridine (1/1) solvent (5 ml). The mixture was stirred for 4 h and then filtered. Orange–red rectangular block crystals of (I) were obtained after about one month by evaporating the filtrate in air.

Crystal data

$[Ni(C_{18}H_{12}N_2O_3)(C_5H_5N)]$	D_x = 1.553 Mg m^{-3}
M_r = 442.11	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3286 reflections
a = 11.768 (4) Å	θ = 2.4–25.5°
b = 8.164 (3) Å	μ = 1.06 mm^{-1}
c = 20.428 (7) Å	T = 298 (2) K
β = 105.474 (6)°	Rectangular block, orange–red
V = 1891.5 (12) Å^3	0.42 × 0.18 × 0.13 mm
Z = 4	

Data collection

Siemens SMART CCD area-detector diffractometer	3321 independent reflections
	2558 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.048
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 25.0°
	$h = -10 \rightarrow 14$
T_{min} = 0.665, T_{max} = 0.875	$k = -9 \rightarrow 9$
9346 measured reflections	$l = -24 \rightarrow 23$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0172P)^2 + 0.829P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.038	
$wR(F^2)$ = 0.092	
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
3321 reflections	$\Delta\rho_{max}$ = 0.56 e Å^{-3}
271 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
H-atom parameters constrained	

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N2	0.82	1.86	2.591 (3)	147

All H atoms were allowed to ride on their parent atoms, with C—H = 0.93 Å and O—H = 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C,O).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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*.

The authors acknowledge the support of the Natural Science Foundation of Shandong Province, People's Republic of China (grant No. Y2003B01).

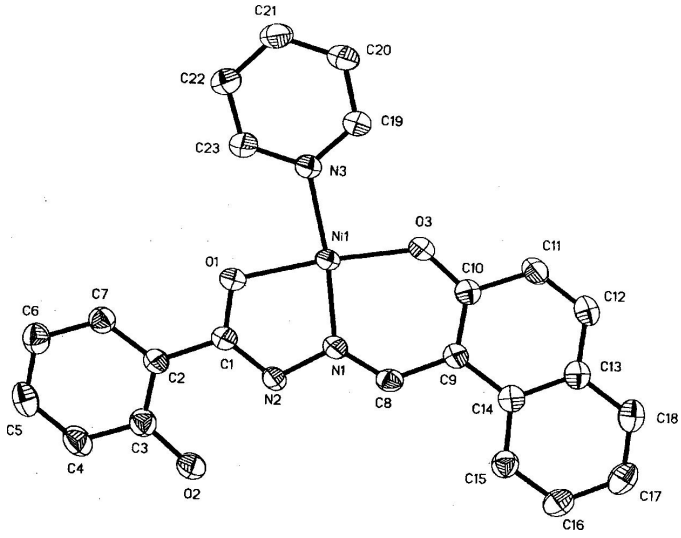


Figure 1
The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted.

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