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## Key indicators

Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$   
 $R$  factor = 0.030  
 $wR$  factor = 0.064  
Data-to-parameter ratio = 12.2

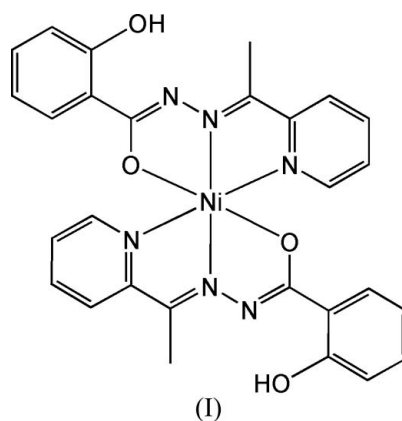
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Bis[*N*-(2-hydroxybenzoyl)-*N'*-[1-(2-pyridyl)-ethylidene]hydrazinato}nickel(II)

The title complex,  $[\text{Ni}(\text{C}_{14}\text{H}_{12}\text{N}_3\text{O}_2)_2]$ , consists of two deprotonated 2-acetylpyridine salicylhydrazone ligands coordinated to the nickel as *N,N',O*-tridentate ligands, forming a neutral complex. The Ni atom lies on a twofold rotation axis. The structure is stabilized by intramolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonding and  $\pi-\pi$  stacking interactions between the pyridyl and benzene rings, leading to a two-dimensional network in the crystal structure.

## Comment

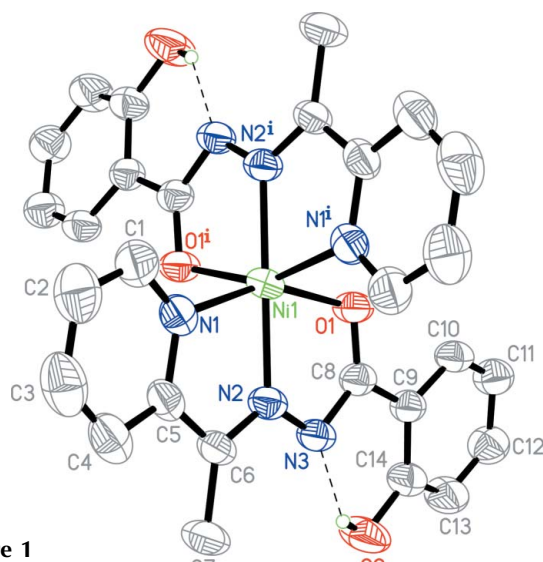
Diazine Schiff base ligands with two coordination compartments linked by a single N—N bridge are employed for their ease of synthesis and high yield in a single-step reaction from commercial and inexpensive reagents (Grove *et al.*, 2004; Bai *et al.*, 2006). The most notable feature of this type of polydentate ligand is that the single N—N bridge of the diazine fragment can rotate freely (Xu *et al.*, 2000; Zhao *et al.*, 2004) so that it usually leads to a situation where a variety of different structural types, such as chains, metallomacrocycles, and metallocrowns are observed when the ligands combine with metals (Bai *et al.*, 2005; Song *et al.*, 2004). On the other hand, the self-assembly of transition metal with diazine ligands introduces many special functional properties, such as magnetism and redox activity, into the structure apart from their particular structural features (Leininger *et al.*, 2000). In our previous work, a mononuclear copper(II) complex generated from the ligand 2-acetylpyridine salicylhydrazone ( $\text{H}_2\text{L}$ ) was reported (Dang *et al.*, 2006). Here, a new mononuclear complex of nickel(II) was constructed *via* self-assembly using the same ligand.



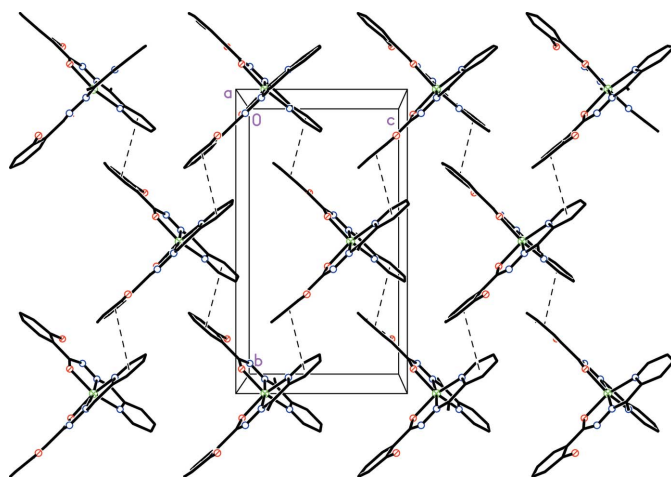
Reaction of  $\text{NiCl}_2\cdot 6\text{H}_2\text{O}$  with the pentadentate Schiff base ligand 2-acetylpyridine salicylhydrazone ( $\text{H}_2\text{L}$ ) leads to the formation of the title nickel(II) complex, (I), which consists of

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**Figure 1**  
View of the molecular structure of the title complex, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms other than the hydroxyl proton have been omitted for clarity. Hydrogen bonds are indicated by dashed lines. [Symmetry code (i)  $-x + 2, -y + 1, z$ .]



**Figure 2**  
Intermolecular  $\pi$ - $\pi$  stacking (dashed lines) in the title complex, viewed along the  $a$  axis. H atoms have been omitted for clarity.

two  $HL^-$  ligands coordinated to the nickel as  $N,N',O$ -tridentate ligands, forming a neutral complex (Fig. 1). The structure is similar to that found for the related copper(II) complex (Dang *et al.*, 2006). The Ni atom lies on a twofold rotation axis and is coordinated in a distorted octahedral configuration by two carbonyl O atoms, two imine N atoms and two pyridine N atoms. Just as has been found in the copper(II) complex, the ligands bond to the nickel in the *mer* configuration with pairs of carbonyl O atoms and pyridyl N atoms each bearing a *cis* relationship, whereas the imino N atoms are *trans* to each other. Intramolecular hydrogen bonds between imino N atoms and hydroxy groups stabilize the molecule. In the crystal structure, molecules are connected together by  $\pi$ - $\pi$  interactions between the benzene and pyridine rings, generating a two-dimensional network (Fig. 2). The dihedral angle and the

centroid-centroid distance between the interacting pair are  $10.8(1)^\circ$  and  $3.859(1) \text{ \AA}$ , respectively.

## Experimental

All chemicals were of reagent grade quality obtained from commercial sources and used without further purification. The ligand  $H_2L$  was synthesized according to the literature methods (Dang *et al.*, 2006). A solution of  $H_2L$  (0.025 g, 0.1 mmol) and  $Et_3N$  (0.011 g, 0.1 mmol) in methanol (6 ml) was layered onto a solution of DMF (6 ml) containing  $NiCl_2 \cdot 6H_2O$  (0.024 g, 0.1 mmol) at the bottom. The solutions were allowed to stand for few weeks at room temperature in darkness, giving X-ray quality crystals (yield, 85%). Analysis calculated for  $C_{28}H_{24}N_6NiO_4$ : C 59.3, H 4.3, N 14.8%; found: C 59.3, H 4.4, N 14.2%.

## Crystal data

$[Ni(C_{14}H_{12}N_3O_2)_2]$	$Z = 4$
$M_r = 567.24$	$D_x = 1.531 \text{ Mg m}^{-3}$
Orthorhombic, $Aba2$	Mo $K\alpha$ radiation
$a = 12.495(3) \text{ \AA}$	$\mu = 0.84 \text{ mm}^{-1}$
$b = 18.672(4) \text{ \AA}$	$T = 293(2) \text{ K}$
$c = 10.549(2) \text{ \AA}$	Block, green
$V = 2461.2(9) \text{ \AA}^3$	$0.20 \times 0.18 \times 0.15 \text{ mm}$

## Data collection

Bruker SMART CCD area-detector diffractometer	2171 independent reflections
$\phi/\omega$ scans	1934 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{int} = 0.041$
5887 measured reflections	$\theta_{max} = 25.0^\circ$

## Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.028P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.030$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.064$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.31 \text{ e \AA}^{-3}$
2171 reflections	$\Delta\rho_{min} = -0.16 \text{ e \AA}^{-3}$
178 parameters	Absolute structure: Flack (1983),
H-atom parameters constrained	1011 Friedel pairs
	Flack parameter: $-0.033(16)$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Ni1—N2	1.9830 (19)	Ni1—O1	2.0977 (19)
Ni1—N1	2.081 (2)		
N2—Ni1—N2 <sup>i</sup>	173.24 (16)	N1—Ni1—O1	154.31 (7)
N2—Ni1—N1 <sup>i</sup>	107.31 (9)	N2—Ni1—O1 <sup>i</sup>	98.26 (8)
N2—Ni1—N1	77.65 (10)	N1—Ni1—O1 <sup>i</sup>	93.59 (8)
N1 <sup>i</sup> —Ni1—N1	89.53 (12)	O1—Ni1—O1 <sup>i</sup>	94.52 (11)
N2—Ni1—O1	77.08 (8)		

Symmetry code: (i)  $-x + 2, -y + 1, z$ .

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O2—H2B $\cdots$ N3	0.82	1.82	2.541 (3)	146

H atoms bonded to C and O atoms were constrained to ride on their parent atoms, with distances of 0.96 (CH<sub>3</sub>), 0.93 (aromatic) and

0.82 Å (OH), and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for CH<sub>3</sub>,  $1.2U_{\text{eq}}(\text{C})$  for aromatic and  $1.2U_{\text{eq}}(\text{O})$  for OH.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINTE* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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