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## Bis(acetato-O)tetrakis(imidazole-*N*<sup>3</sup>)-nickel(II)

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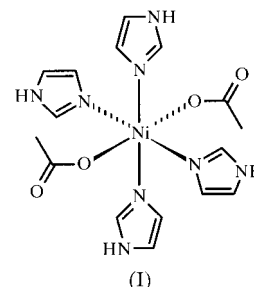
In the title compound,  $[\text{Ni}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_3\text{H}_4\text{N}_2)_4]$ , the Ni atom is coordinated centrosymmetrically by four N and two O atoms in an octahedral coordination [Ni–N = 1.986 (3) and 2.054 (3) Å; Ni–O = 2.697 (3) Å]. The O atoms of the acetate anions form hydrogen bonds to adjacent imidazole moieties, with the free O atom forming a somewhat shorter bond [N··O = 2.679 (3) and 2.870 (4) Å]. The hydrogen bonds give rise to a two-dimensional layer structure.

### Comment

Interest in the chemistry of transition metal complexes of imidazole and substituted imidazoles stems from attempts to model the binding site of the histidine residue in metallo-proteins (Henriksson, 1977; Povse *et al.*, 1998; Wang *et al.*, 2000). The structures of the complexes constitute the primary source of input data for semi-empirical theoretical modeling of metal–DNA and metal–protein interactions (Abuhijleh & Woods, 1992). The copper(II) systems have been most well documented (Abuhijleh & Woods, 1992; Fransson & Lundberg, 1972; Henriksson, 1977; Lundberg, 1972). Following the synthesis of the hexakis(imidazole)nickel(II) halides (Eilbeck *et al.*, 1967), other hexakis(imidazole)nickel adducts were prepared and structurally characterized (Konopelski *et al.*, 1976; Perec *et al.*, 1999; Povse *et al.*, 1998; Santoro *et al.*, 1969; van Ingen Schenau, 1975; Wang *et al.*, 2000). Four imidazole ligands pack around the Ni atom in tetrakis(imidazole-*N*<sup>3</sup>)-cyanate (Koman *et al.*, 1991), whose Ni atom shows octahedral coordination.

With the acetate ion as the counter-ion, only four imidazole ligands pack around the Ni atom in the title compound, bis(-acetato-O)tetrakis(imidazole-*N*<sup>3</sup>)nickel(II), (I), which is isostructural with the copper analog (Abuhijleh & Woods, 1992). As expected, the Ni–N distances are shorter than those found in the six-coordinate hexakis and the four-coordinate tetrakis compounds (See *et al.*, 1998). The six-coordi-

nate geometry arises from two relatively long Ni–O distances [2.697 (3) Å]; the bonds are somewhat longer than the Jahn–Teller elongated bonds in the copper analog (Abuhijleh & Woods, 1992). The acetate groups permit the imidazole ligands



to approach the metal atom closer than the isothiocyanate ions in the nickel isothiocyanate adduct (Koman *et al.*, 1991) and the water molecules in the dihydrated nickel saccharinate adduct (Zhang *et al.*, 1992).

The negative charge is delocalized over the acetate ions; both O atoms form hydrogen bonds to adjacent imidazole moieties. The uncoordinated O atom is engaged in a somewhat stronger hydrogen bond [N··O = 2.679 (3) and 2.870 (4) Å]. Hydrogen bonding gives rise to a two-dimensional layered structure.

### Experimental

Nickel acetate and imidazole (1:4 stoichiometry) were heated in *n*-propanol to furnish the title compound as an oil after the solvent had been removed. The solid compound was obtained as crystals after recrystallization from absolute ethanol.

#### Crystal data

$[\text{Ni}(\text{C}_2\text{H}_3\text{O}_2)_2(\text{C}_3\text{H}_4\text{N}_2)_4]$   
 $M_r = 449.13$   
Monoclinic,  $C2/c$   
 $a = 13.46$  (2) Å  
 $b = 8.62$  (1) Å  
 $c = 17.89$  (2) Å  
 $\beta = 105.28$  (1)°  
 $V = 2001$  (4) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.491$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 3146 reflections  
 $\theta = 2.36$ – $26.00$ °  
 $\mu = 1.010$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
Parallelepiped, pale blue  
 $0.25 \times 0.25 \times 0.20$  mm

#### Data collection

MarResearch Image Plate diffractometer  
Method: 95 frames at 2° intervals, counting time 2 min.  
3146 measured reflections  
1842 independent reflections  
1540 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$   
 $\theta_{\text{max}} = 26.00$ °  
 $h = 0 \rightarrow 16$   
 $k = -10 \rightarrow 10$   
 $l = -21 \rightarrow 21$   
Intensity decay: none

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.105$   
 $S = 1.063$   
1842 reflections  
135 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0629P)^2 + 1.9165P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.52$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.34$  e Å<sup>-3</sup>  
Extinction correction: SHELXL97  
Extinction coefficient: 0.009 (1)

**Table 1**

Selected geometric parameters (Å, °).

Ni1—N1	1.986 (3)	Ni1—N3 <sup>i</sup>	2.054 (3)
Ni1—N1 <sup>i</sup>	1.986 (3)	Ni1—O1	2.697 (3)
Ni1—N3	2.054 (3)	Ni1—O1 <sup>i</sup>	2.697 (3)
N1—Ni1—N1 <sup>i</sup>	180.0	N1 <sup>i</sup> —Ni1—O1 <sup>i</sup>	91.8 (1)
N1—Ni1—N3	89.3 (1)	N3—Ni1—N3 <sup>i</sup>	180.0
N1—Ni1—N3 <sup>i</sup>	90.7 (1)	N3—Ni1—O1	95.4 (1)
N1—Ni1—O1	91.8 (1)	N3—Ni1—O1 <sup>i</sup>	84.6 (1)
N1—Ni1—O1 <sup>i</sup>	88.2 (1)	N3 <sup>i</sup> —Ni1—O1	84.6 (1)
N1 <sup>i</sup> —Ni1—N3	90.7 (1)	N3 <sup>i</sup> —Ni1—O1 <sup>i</sup>	95.4 (1)
N1 <sup>i</sup> —Ni1—N3 <sup>i</sup>	89.3 (1)	O1—Ni1—O1 <sup>i</sup>	180.0 (1)
N1 <sup>i</sup> —Ni1—O1	88.2 (1)		

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

**Table 2**

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2 $\cdots$ O2 <sup>i</sup>	0.86	1.82	2.679 (3)	175
N4—H4 $\cdots$ O1 <sup>ii</sup>	0.86	2.01	2.870 (4)	175

Symmetry codes: (i)  $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$ ; (ii)  $\frac{1}{2} + x, \frac{1}{2} + y, z$ .

Distances involving H atoms were constrained to N—H = 0.86 Å and C—H = 0.93–0.96 Å.

Data collection: *XDS* (Kabsch, 1988); cell refinement: *XDS*; data reduction: *XDS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97*

(Sheldrick, 1997); software used to prepare material for publication: *SHELXL97*.

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