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Diaquabis(imidazole-κ*N*)bis(nitrobenzoato-κ*O*)nickel(II)

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The title complex, $[Ni(C_7H_4NO_4)_2(C_3H_4N_2)_2(H_2O)_2]$, assumes an octahedral coordination geometry with the Ni atom located on an inversion centre. The overlapped arrangement and the separation of 3.535 (14) Å suggest the existence of π–π stacking between parallel imidazole ligands. Both intramolecular and intermolecular hydrogen bonding occur between imidazole, coordinated water molecules and the carboxyl group.

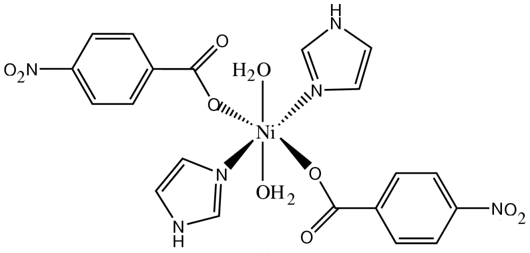
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.026
wR factor = 0.068
Data-to-parameter ratio = 15.0

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

Comment

π–π stacking between aromatic rings is related to the electron transfer process in some biological systems (Deisenhofer & Michel, 1989). Aromatic polycyclic compounds such as phenanthroline, benzimidazole and quinoline have shown π–π stacking in metal complexes. As a part of our investigations of π–π stacking in metal complexes (Chen *et al.*, 2003), imidazole has been used to prepare a series of metal complexes in the laboratory.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The Ni^{2+} atom, located on an inversion center, assumes an octahedral coordination geometry formed by two imidazole molecules, two water molecules and two nitrobenzoate anions, with normal bond distances and angles (see Table 1). The

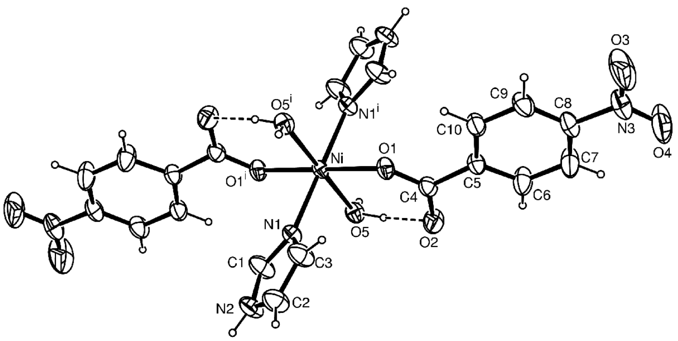


Figure 1
The molecular structure of (I) with 50% probability displacement ellipsoids. Dashed lines indicate the hydrogen bonding. [Symmetry code: (i) $1 - x, 1 - y, 1 - z$.]

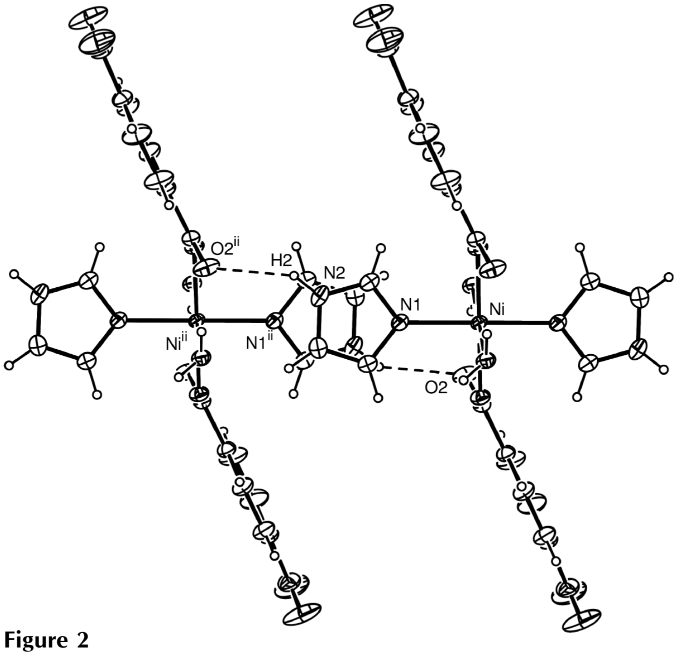


Figure 2
A diagram showing the π–π stacking between imidazole rings. Dashed lines indicate the hydrogen bonding between imidazole and carboxyl groups. [Symmetry code: (ii) $1 - x, 2 - y, 1 - z$.]

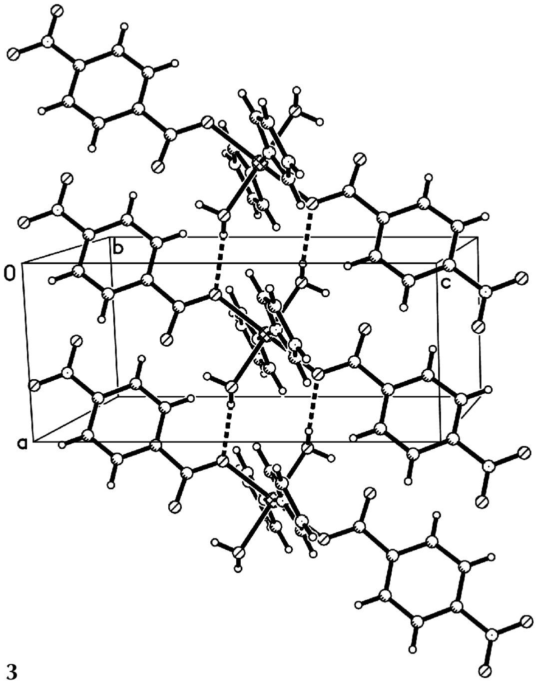


Figure 3
A molecular packing diagram. Dashed lines indicate intermolecular hydrogen bonding between coordinated water and carboxyl groups.

carboxyl group of the nitrobenzoate coordinates to the Ni^{2+} atom in monodentate mode, and the uncoordinated carboxyl O atom is intramolecularly hydrogen bonded to the adjacent coordinated water (Fig. 1) and intermolecularly hydrogen bonded to the imidazole of a neighboring complex molecule (see Fig. 2).

An overlapped arrangement of parallel imidazole ligands in neighboring complex molecules is observed in the crystal (Fig. 2). The imidazole rings related by a symmetry transformation $(1 - x, 2 - y, 1 - z)$ are separated by 3.535 (14) Å. These findings suggest the existence of a π–π stacking interaction between imidazole rings.

The coordinated water molecule links with a neighboring complex molecule *via* an O—H$\cdots$O hydrogen bond (Fig. 3). Weak C—H$\cdots$O hydrogen bonding occurs in the crystal structure (Table 2).

Experimental

$NiCl_2\cdot 6H_2O$ (0.24 g, 1 mmol) was dissolved in an aqueous solution (10 ml) containing nitrobenzoic acid (0.33 g, 2 mmol) and NaOH (0.08 g, 2 mmol). After the solution was refluxed for 15 min, an ethanol solution (10 ml) of imidazole (0.14 g, 2 mmol) was added with continuous stirring. The resulting solution was refluxed for 2 h and filtered. Green single crystals were obtained from the filtrate after 3 d.

Crystal data

$[Ni(C_7H_4NO_4)_2(C_3H_4N_2)_2(H_2O)_2]$
$M_r = 563.13$
Triclinic, $P\overline{1}$
$a = 5.644$ (2) Å
$b = 8.0547$ (18) Å
$c = 12.716$ (2) Å
$\alpha = 75.032$ (13)°
$\beta = 87.759$ (13)°
$\gamma = 87.079$ (12)°
$V = 557.5$ (3) Å^3

$Z = 1$
$D_x = 1.677$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2370 reflections
$\theta = 3.4$–27.0°
$\mu = 0.94$ mm^{-1}
$T = 295$ (2) K
Prism, green
0.27 × 0.18 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.770$, $T_{max} = 0.855$
5338 measured reflections

2527 independent reflections
2413 reflections with $I > 2\sigma(I)$
$R_{int} = 0.013$
$\theta_{max} = 27.4°$
$h = -7 \rightarrow 6$
$k = -10 \rightarrow 10$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.068$
$S = 1.09$
2527 reflections
169 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0349P)^2 + 0.2032P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni—N1	2.0602 (13)	Ni—O1	2.1371 (10)
Ni—O5	2.0961 (11)		
N1—Ni—O5	88.78 (5)	O5—Ni—O1	93.68 (4)
N1—Ni—O1	92.80 (5)		

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^{ii}	0.86	2.33	3.074 (2)	146
O5—H5*A*$\cdots$O2	0.87	1.79	2.6304 (18)	162
O5—H5*B*$\cdots$O1^{iii}	0.81	2.11	2.8813 (17)	159
C3—H3$\cdots$O5^{iv}	0.93	2.37	3.278 (2)	166

Symmetry codes: (ii) $1 - x, 2 - y, 1 - z$; (iii) $x - 1, y, z$; (iv) $1 + x, y, z$.

H atoms on the water molecule were located in a difference Fourier map and included in structure-factor calculations with fixed coordinates and isotropic displacement parameters set to 0.05 Å^2. Other H atoms were placed in calculated positions with C—H = 0.93 Å and N—H = 0.86 Å, and were included in the final cycles of refinement in a riding model, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$ of the carrier atoms.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *XP* (Siemens, 1994).

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