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**Key indicators**

Single-crystal X-ray study  
 T = 293 K  
 Mean  $\sigma(C-C)$  = 0.005 Å  
 R factor = 0.039  
 wR factor = 0.103  
 Data-to-parameter ratio = 9.8

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

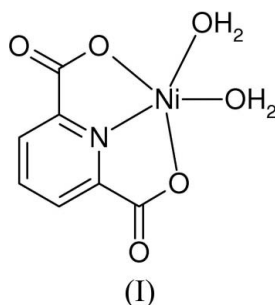
**Diaqua(pyridine-2,6-dicarboxylato)nickel(II)**

The title compound,  $[Ni(C_7H_3NO_4)(H_2O)_2]$ , has been prepared by the hydrothermal reaction of nickel(II) chloride and pyridine-2,6-dicarboxylic acid. It is isostructural with the analogous  $Cu^{II}$  complex.

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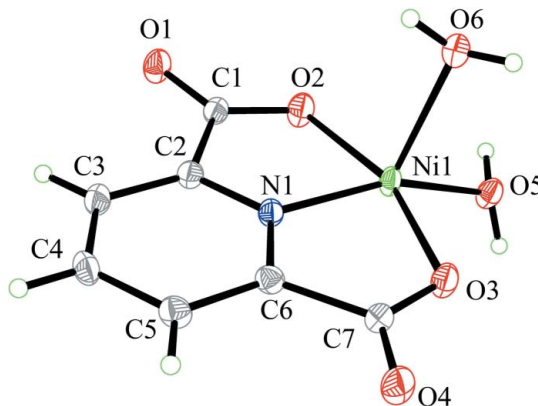
**Comment**

The title compound, (I), is isostructural with its  $Cu^{II}$  analogue (Sileo *et al.*, 1997; Koman *et al.*, 2001; Wang *et al.*, 2003). The  $Ni^{II}$  atom is pentacoordinated in an approximately square-pyramidal geometry (Table 1), chelated by two O atoms and one N atom from the pyridine-2,6-dicarboxylate ligand, and two water molecules (Fig. 1). Hydrogen bonds between the water molecules and the O atoms of the carboxyl groups (Table 2) link the molecules into layers in the *ac* planes (Fig. 2).



**Experimental**

A mixture of nickel(II) chloride (0.5 mmol), potassium hydroxide (0.5 mmol), pyridine-2,6-dicarboxylic acid (0.5 mmol) and  $H_2O$  (8 ml) in a 25 ml Teflon-lined stainless steel autoclave was heated at



**Figure 1**  
 The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level for non-H atoms.

413 K for 2 d, and then cooled to room temperature. Green block-shaped crystals of (I) were obtained with a yield of 36%. Elemental analysis found: C 32.16, H 2.45, N 5.22, O 24.66, Ni 24.32%; calculated: C 32.33, H 2.69, N 5.39, O 24.63, Ni 24.46%

#### Crystal data

$[\text{Ni}(\text{C}_7\text{H}_3\text{NO}_4)(\text{H}_2\text{O})_2]$	$V = 426.51(6) \text{ \AA}^3$
$M_r = 259.85$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 2.023 \text{ Mg m}^{-3}$
$a = 4.7042(4) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 8.9656(7) \text{ \AA}$	$\mu = 2.28 \text{ mm}^{-1}$
$c = 10.3228(8) \text{ \AA}$	$T = 293(2) \text{ K}$
$\alpha = 81.103(2)^\circ$	Block, green
$\beta = 85.720(2)^\circ$	$0.40 \times 0.37 \times 0.33 \text{ mm}$
$\gamma = 83.333(2)^\circ$	

#### Data collection

Bruker SMART CCD diffractometer	2247 measured reflections
$\varphi$ and $\omega$ scans	1507 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1328 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.418$ , $T_{\max} = 0.471$	$R_{\text{int}} = 0.024$
	$\theta_{\text{max}} = 25.1^\circ$

#### Refinement

Refinement on $F^2$	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.039$	
$wR(F^2) = 0.103$	$w = 1/[\sigma^2(F_o^2) + (0.0709P)^2]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
1507 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
153 parameters	$\Delta\rho_{\text{max}} = 0.63 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.74 \text{ e \AA}^{-3}$

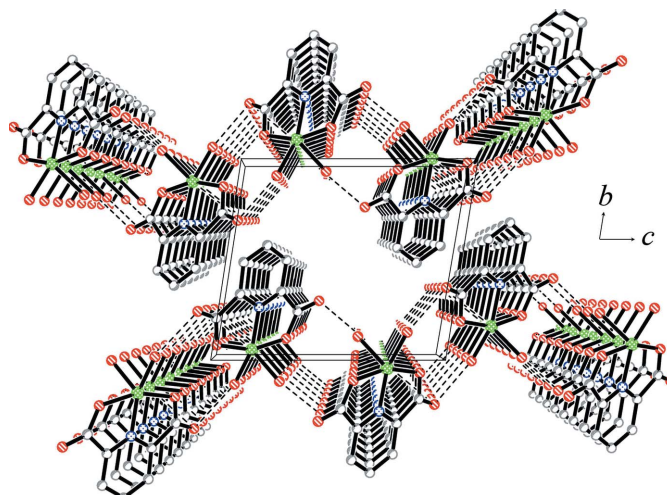
**Table 1**

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

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
O5—H51 $\cdots$ O1 <sup>i</sup>	0.89 (3)	1.85 (3)	2.729 (4)	167 (6)
O5—H52 $\cdots$ O2 <sup>ii</sup>	0.89 (3)	2.22 (5)	2.970 (4)	142 (6)
O6—H62 $\cdots$ O3 <sup>iii</sup>	0.89 (3)	1.95 (3)	2.759 (4)	150 (4)
O6—H61 $\cdots$ O4 <sup>iv</sup>	0.89 (3)	1.84 (3)	2.722 (3)	169 (4)

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

H atoms bound to C atoms were placed in idealized positions and allowed to ride during subsequent refinement, with  $C\text{---}H = 0.93 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . H atoms of the water molecules were located in a difference Fourier map and refined with isotropic displacement parameters. The O—H distances were restrained to a



**Figure 2**

View of (I) along the  $a$ -axis direction, showing hydrogen-bonded layers in the  $ac$  planes. H atoms are omitted and hydrogen bonds are shown as dashed lines.

common refined value, and the  $\text{H}\cdots\text{H}$  distances were restrained to 1.63 times that value. The refined O—H distance is  $0.89(3) \text{ \AA}$ .

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1999); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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