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Key indicators

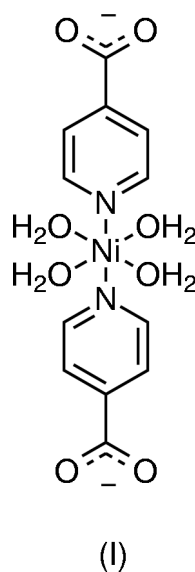
Single-crystal X-ray study
 $T = 123\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.025
 wR factor = 0.058
Data-to-parameter ratio = 13.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*trans*-Tetraaquabis(pyridine-4-carboxylate- κN)-
nickel(II)

The title complex, $[\text{Ni}(\text{C}_6\text{H}_4\text{NO}_2)_2(\text{H}_2\text{O})_4]$, consists of Ni atoms coordinated to two *trans* pyridylcarboxylate ligands, coordinated through the N atoms, and four water ligands. The Ni atom lies on a centre of symmetry. Extensive inter-complex hydrogen bonding occurs between the water ligands and the carboxylate groups, resulting in a three-dimensional network.

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Comment

Pyridinecarboxylate ligands have recently been used in the construction of novel coordination polymers with interesting microporous and non-linear optical properties (Lin *et al.*, 1998; Evans, Xiong *et al.*, 1999; Evans, Wang *et al.*, 1999; Evans & Lin, 2000). A feature of this class of bridging ligand is the presence of two different coordinating functionalities – a pyridyl group and a carboxylate group. The ligands also offer the possibility of participating in hydrogen-bonding networks if monodentate coordination occurs. We report here the structure of $\text{NiL}_2(\text{H}_2\text{O})_4$ (L is pyridine-4-carboxylate), (I), in which such a hydrogen-bonded network is found.



The structure of (I) is isomorphous with the previously reported manganese(II) (Hauptmann *et al.*, 2000), iron(II) (Liu *et al.*, 1999), cobalt(II) (Waizumi *et al.*, 1998), copper(II) (Okabe *et al.*, 1993; Waizumi *et al.*, 1998), zinc(II) (Cingi *et al.*, 1971) and cadmium(II) (Cingi *et al.*, 1971) structures. It consists of mononuclear nickel complexes in which the metal ion is coordinated to the N atoms of two *trans* pyridine-4-carboxylate ligands, and to four water ligands (Fig. 1). The octahedrally coordinated Ni atom (Table 1) lies on a centre of

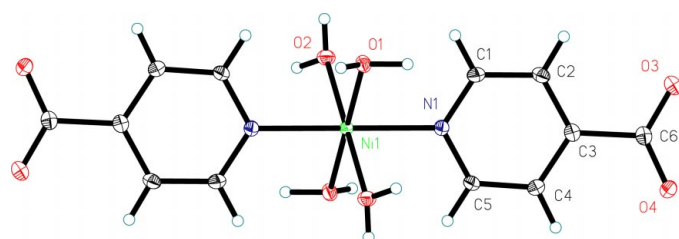


Figure 1
Atom-numbering scheme for (I). Displacement ellipsoids are drawn at the 50% probability level.

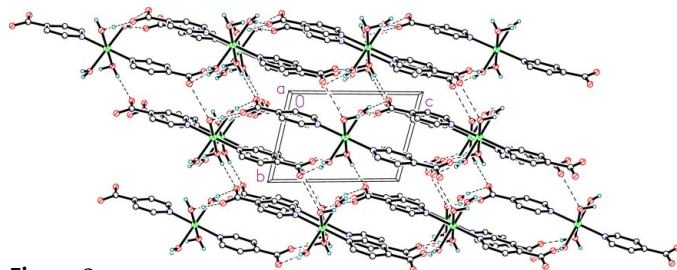


Figure 2
Crystal packing in (I), showing the extensive hydrogen bonding between complexes.

symmetry. The carboxylate group of the ligand is twisted slightly from the plane of the pyridyl group [the angle between the two planes is $13.93(8)^\circ$].

Extensive hydrogen bonding between the water ligands and the uncoordinated carboxylate groups generates a complex three-dimensional network (Fig. 2). Each carboxylate O atom is hydrogen bonded to two separate water ligands (Table 2), and each water ligand hydrogen bonds to two separate carboxylates. Each complex is thus connected to six neighbours *via* 16 O—H...O hydrogen bonds.

Experimental

The title compound was obtained from an aqueous solution containing nickel nitrate, sodium dicyanamide and pyridine-4-carboxylic acid.

Crystal data

$[\text{Ni}(\text{C}_6\text{H}_4\text{NO}_2)_2(\text{H}_2\text{O})_4]$	$Z = 1$
$M_r = 374.98$	$D_x = 1.822 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 6.2862(3) \text{ \AA}$	Cell parameters from 3694 reflections
$b = 6.8598(2) \text{ \AA}$	$\theta = 2.3\text{--}28.3^\circ$
$c = 9.2394(4) \text{ \AA}$	$\mu = 1.468 \text{ mm}^{-1}$
$\alpha = 96.511(3)^\circ$	$T = 123(2) \text{ K}$
$\beta = 104.929(2)^\circ$	Plate, blue
$\gamma = 113.692(3)^\circ$	$0.18 \times 0.13 \times 0.05 \text{ mm}$
$V = 341.77(2) \text{ \AA}^3$	

Data collection

Nonius KappaCCD diffractometer	1558 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.029$
Absorption correction: by integration (XPREP; Siemens, 1994)	$\theta_{\text{max}} = 28.3^\circ$
$T_{\text{min}} = 0.835$, $T_{\text{max}} = 0.940$	$h = -8 \rightarrow 8$
3694 measured reflections	$k = -8 \rightarrow 8$
1626 independent reflections	$l = -11 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0023P)^2 + 0.1806P]$
$R[F^2 > 2\sigma(F^2)] = 0.025$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.058$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.15$	$\Delta\rho_{\text{max}} = 0.34 \text{ e \AA}^{-3}$
1626 reflections	$\Delta\rho_{\text{min}} = -0.52 \text{ e \AA}^{-3}$
122 parameters	
H atoms: see below	

Table 1

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

Ni1—O1	2.0669 (11)	Ni1—O2	2.0932 (11)
Ni1—N1	2.0891 (13)		
O1—Ni1—N1	91.90 (5)	N1—Ni1—O2	90.76 (5)
O1—Ni1—O2	93.24 (5)		

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O1—H11...O4 ⁱ	1.00 (2)	1.64 (2)	2.634 (2)	177 (2)
O1—H12...O3 ⁱⁱ	0.80 (2)	2.00 (3)	2.793 (2)	172 (2)
O2—H21...O3 ⁱⁱⁱ	0.83 (3)	2.00 (3)	2.825 (2)	171 (2)
O2—H22...O4 ^{iv}	0.83 (3)	1.96 (3)	2.786 (2)	178 (3)

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

All H atoms were observed in difference syntheses, however only those of the water ligands were allowed to refine freely.

Data collection: *COLLECT* (Hooft, 1998); cell refinement and data reduction: *DENZO-SMN* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

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