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trans-Tetraaquabis(pyridine-3-carboxylate-κN)-nickel(II)

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Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.004 Å
R factor = 0.032
wR factor = 0.058
Data-to-parameter ratio = 12.1

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

The title complex, $[Ni(C_6H_4NO_2)_2(H_2O)_4]$, consists of an Ni atom coordinated to two *trans* pyridinecarboxylate ligands, coordinated through the N atoms, and four water ligands. The Ni atom lies on a site of 2/*m* symmetry, and the pyridinecarboxylate ligand lies on a mirror plane. Extensive inter-complex hydrogen bonding occurs between the water ligands and the carboxylate groups, resulting in a three-dimensional network.

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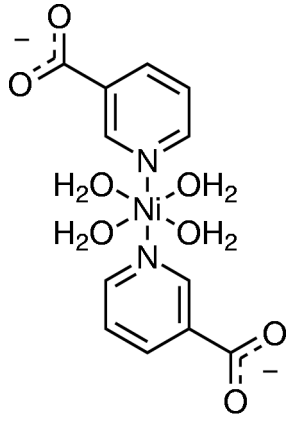
Comment

A number of novel coordination polymers which contain bridging pyridinecarboxylate ligands and display interesting physical properties have been reported recently (Lin *et al.*, 1998; Evans, Xiong *et al.*, 1999; Evans, Wang *et al.*, 1999; Evans & Lin, 2000). However, if the ligands coordinate only in a monodentate fashion, the possibility of participating in hydrogen bonding-networks arises. We report here the structure of $NiL_2(H_2O)_4$ (L is pyridine-3-carboxylate), (I), in which such a hydrogen-bonded network is found.



(I)

The structure of (I) is isomorphous with the previously reported cobalt(II) (Anagnostopoulos *et al.*, 1969; Waizumi *et al.*, 1998) and zinc(II) (Cotton *et al.*, 1991; Cingi *et al.*, 1971; Sabirov *et al.*, 1984) analogues. It consists of mononuclear nickel complexes containing two *trans* nitrogen-bound pyridine-3-carboxylate ligands and four water ligands (Fig. 1). The octahedrally coordinated Ni atom (Table 1) lies on a site of 2/*m* symmetry, while the pyridinecarboxylate ligand lies on a mirror plane and is thus rigidly planar.

As expected, there is extensive hydrogen bonding between the water ligands and the uncoordinated carboxylate groups, giving rise to a complex three-dimensional network (Fig. 2).

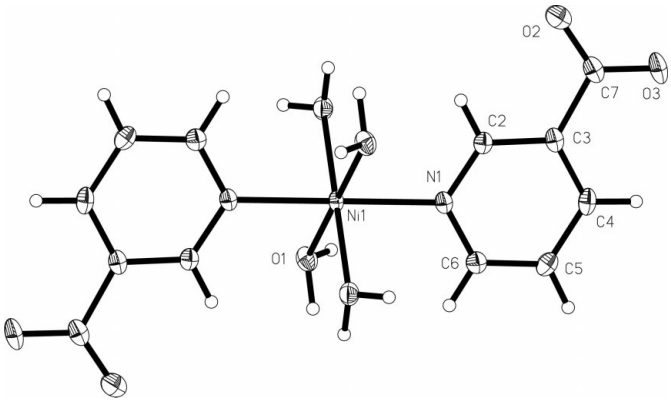


Figure 1
Atom-numbering scheme for (I). Displacement ellipsoids are drawn at the 50% probability level.

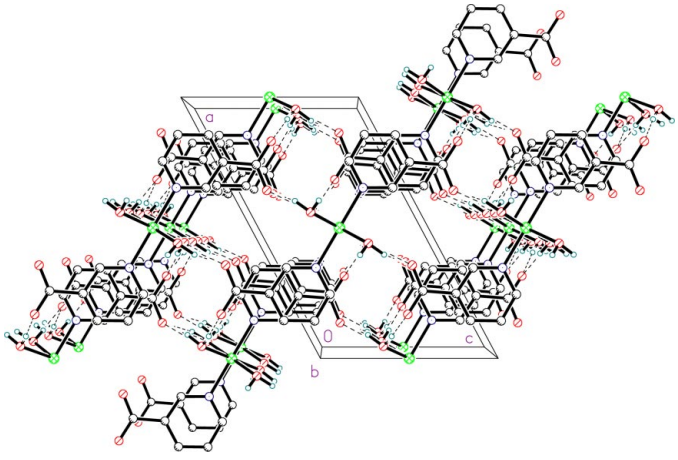


Figure 2
Crystal packing in (I), showing the extensive hydrogen bonding between complexes.

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 thus participates in 16 O—H···O intermolecular hydrogen bonds to six neighbouring complexes.

Experimental

The title compound was obtained from an aqueous solution containing nickel nitrate, sodium dicyanamide and pyridine-3-carboxylic acid.

Crystal data

$[Ni(C_6H_4NO_2)_2(H_2O)_4]$
M_r = 374.98
Monoclinic, *C*2/*m*
a = 14.0549 (7) Å
b = 6.8170 (2) Å
c = 8.4359 (4) Å
β = 118.137 (2)°
V = 712.74 (5) Å^3
Z = 2
D_x = 1.747 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 5663 reflections
θ = 2.7–27.8°
μ = 1.41 mm^{-1}
T = 123 (2) K
Rod, light blue
0.30 × 0.05 × 0.03 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
5664 measured reflections
916 independent reflections
843 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 27.8°
$h = -18 \rightarrow 18$
$k = -8 \rightarrow 8$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.058
S = 1.12
916 reflections
76 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.0108P)^2 + 1.0314P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	2.0775 (12)	Ni1—N1	2.098 (2)
O1—Ni1—N1	91.32 (5)	O1—Ni1—O1^{i}	91.52 (8)

Symmetry code: (i) *x*, −*y*, *z*.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O2^{i}	0.95 (3)	1.77 (3)	2.696 (2)	161 (2)
O1—H1*B*···O3^{ii}	0.82 (3)	1.89 (3)	2.708 (2)	173 (3)

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

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: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL*97.

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