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Key indicators

Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.032
 wR factor = 0.078
Data-to-parameter ratio = 9.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Tetraaquabis(1-carboxylatomethylpyridinium-4-carboxylato)nickel(II)

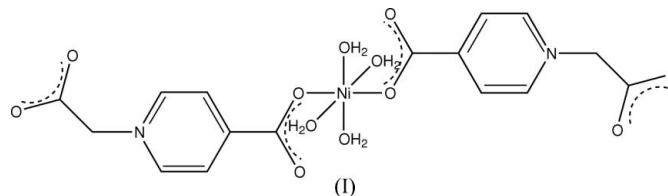
The crystal structure of the title complex, $[\text{Ni}(\text{C}_8\text{H}_6\text{NO}_4)_2(\text{H}_2\text{O})_4]$, consists of discrete Ni^{II} complex molecules, which are linked to each other by classical $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding and offset $\pi-\pi$ stacking interactions. The Ni^{II} atom is octahedrally coordinated by four water molecules lying on the equatorial plane and two monodentate carboxylate groups from two 1-carboxylatomethylpyridinium-4-carboxylate ligands.

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Comment

Coordination chemistry remains a very active field in the structural design of supramolecular chemistry. By virtue of their overall neutral charge and deprotonated carboxyl group, betaine and its derivatives are easily coordinated to metal atoms and can be used to prepare soluble metal complexes. During the preparation of polymeric complexes using 1-carboxymethylpyridine-4-carboxylate (*L*) as a bridging ligand, we obtained crystals of the title monomeric Ni^{II} complex, (I).



In the title complex, (I), four water molecules and two monodentate carboxylate groups from *L* ligands coordinate to Ni^{II} , giving rise to an octahedron, with the four water O atoms in the equatorial plane. The O atom of the carboxylate group not attached to Ni^{II} is hydrogen-bonded to the coordinated water molecules (Fig. 2). There are also weak offset $\pi-\pi$ stacking interactions (Janiak, 2000), as shown in Fig. 2. The interplanar distances between approximately parallel pyridine planes are 3.426 and 3.492 Å, and the centroid-centroid distances between pyridine planes are 3.929 and 3.998 Å, respectively.

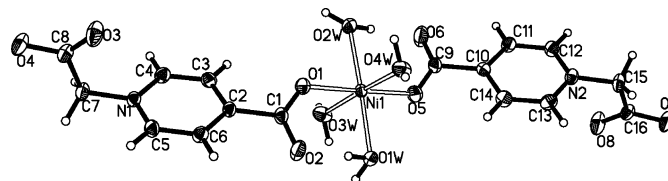


Figure 1

The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as spheres of arbitrary radii.

Experimental

Compound (I) was prepared by reaction of NaL (0.203 g, 1 mmol) and Ni(ClO₄)₂·6H₂O (0.365 g, 1 mmol) in distilled water (5 ml). The solution was stirred for about 6 min at 333 K and then left to stand at room temperature. Single crystals of (I) were obtained after 3 d.

Crystal data

[Ni(C₈H₆NO₄)₂(H₂O)₄]
M_r = 491.05
 Monoclinic, *P*₂₁
a = 6.4670 (5) Å
b = 19.116 (2) Å
c = 7.7037 (16) Å
 β = 92.344 (11)°
V = 951.6 (2) Å³
Z = 2
D_x = 1.714 Mg m⁻³
 Mo *K*α radiation
 μ = 1.09 mm⁻¹
T = 294 (2) K
 Block, green
 0.23 × 0.22 × 0.19 mm

Data collection

Siemens P4 diffractometer
 ω scans
 Absorption correction: ψ scan
 (North *et al.*, 1968)
*T*_{min} = 0.787, *T*_{max} = 0.819
 3383 measured reflections
 2738 independent reflections
 2626 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.020
 θ_{max} = 28.3°
 3 standard reflections
 every 120 reflections
 intensity decay: 8%

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.032
wR(*F*²) = 0.078
S = 1.07
 2738 reflections
 304 parameters
 H atoms treated by a mixture of
 independent and constrained
 refinement
w = 1/[σ²(*F*_o²) + (0.0453*P*)²
 + 0.2043*P*]
 where *P* = (*F*_o² + 2*F*_c²)/3
 (Δ/σ)_{max} = 0.001
 Δρ_{max} = 0.40 e Å⁻³
 Δρ_{min} = -0.52 e Å⁻³
 Absolute structure: Flack (1983),
 with 26 Friedel pairs
 Flack parameter: 0.096 (14)

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1W—H1WA···O2W ⁱ	0.85 (3)	2.24 (3)	2.906 (3)	136 (4)
O1W—H1WB···O8 ⁱⁱ	0.86 (3)	1.84 (3)	2.692 (4)	172 (4)
O2W—H2WA···O1W ⁱⁱⁱ	0.84 (3)	2.07 (3)	2.906 (3)	174 (5)
O2W—H2WB···O3 ^{iv}	0.85 (4)	1.99 (4)	2.835 (4)	173 (5)
O3W—H3WA···O4 ^v	0.86 (4)	1.86 (2)	2.674 (4)	156 (4)
O3W—H3WB···O7 ^{vi}	0.86 (3)	1.90 (2)	2.718 (4)	158 (4)

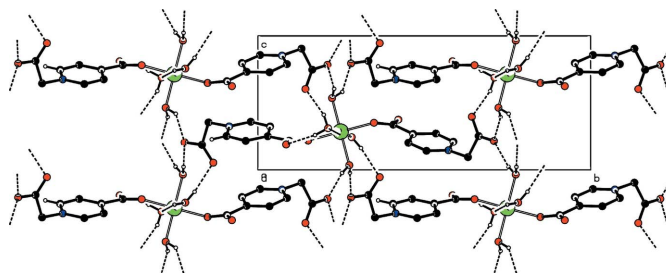


Figure 2

The extended structure of (I), formed through hydrogen-bonding interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O4W—H4WA···O4 ^{iv}	0.85 (3)	1.84 (2)	2.665 (4)	163 (4)
O4W—H4WB···O7 ^{vi}	0.86 (4)	1.97 (3)	2.707 (4)	143 (4)

Symmetry codes: (i) *x* - 1, *y*, *z*; (ii) -*x* - 1, *y* + ½, -*z*; (iii) *x* + 1, *y*, *z*; (iv) -*x* + 1, *y* - ½, -*z* + 1; (v) -*x* + 1, *y* - ½, -*z*; (vi) -*x* - 1, *y* + ½, -*z* + 1.

H atoms attached to C atoms were treated as riding on their parent atoms, with C—H = 0.93 (aromatic) and 0.97 Å (CH₂), and *U*_{iso}(H) = 1.2*U*_{eq}(C). H atoms attached to water molecules were refined using restraints [O—H = 0.85 (1) Å and H···H = 1.45 (2) Å] and with *U*_{iso}(H) = 1.5*U*_{eq}(C).

Data collection: XSCANS (Siemens, 1994); cell refinement: XSCANS; data reduction: XSCANS; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997) and PLATON (Spek, 2003); software used to prepare material for publication: SHELXTL.

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