

Poly[aquabis(μ -pyrazine-2-carboxylato)nickel(II)]Lu-Jiang Hao,^{a*} Chun-Hua Mu^b
and Tian-Tian Liu^a^aCollege of Food and Biological Engineering,
Shandong Institute of Light Industry, Jinan
250353, People's Republic of China, and^bMaize Research Institute, Shandong Academy of
Agricultural Sciences, Jinan 250100, People's
Republic of ChinaCorrespondence e-mail:
lujianghao001@yahoo.com.cn

Key indicators

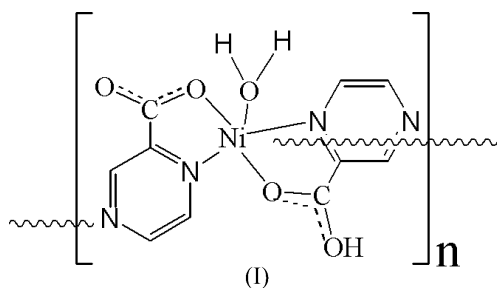
Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.006$ Å
 R factor = 0.034
 wR factor = 0.085
Data-to-parameter ratio = 12.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The asymmetric unit of the title compound, $[\text{Ni}(\text{C}_5\text{H}_3\text{N}_2\text{O}_2)_2(\text{H}_2\text{O})]_n$, contains two bidentate pyrazine-2-carboxylate anions bonded to Ni^{II} in the equatorial plane through one N and one O atom. The Ni^{II} atoms are linked into chains by the second N atom of one of the pyrazine-2-carboxylate anions bonding to an axial site of a neighbouring Ni^{II} atom. The slightly distorted octahedral coordination around Ni^{II} is completed by a water molecule, which forms hydrogen bonds linking the chains into a three-dimensional structure.

Received 8 December 2006
Accepted 13 December 2006

Comment

In recent years, carboxylic acids have been widely used as polydentate ligands which can coordinate to transition or rare earth ions yielding complexes with interesting properties that are useful in materials science (Church & Halvorson, 1959; Chung *et al.*, 1971) and in biological systems (Okabe & Oya, 2000; Serre *et al.*, 2005; Pocker & Fong, 1980; Scapin *et al.*, 1997). For example, Kim *et al.* (2001) focused on the syntheses of transition metal complexes containing benzenecarboxylate and rigid aromatic pyridine ligands in order to study their electronic conductivity and magnetic properties. The importance of transition metal dicarboxylate complexes prompted us to pursue synthetic strategies for these compounds, using pyrazine-2-carboxylate as a polydentate ligand. Here we report the synthesis and X-ray crystal structure analysis of the title compound, (I).



The Ni^{II} atom of (I) is coordinated in a bidentate fashion by two O and two N atoms from two independent pyrazine-2-carboxylate anions. The distorted octahedral coordination is completed by another N atom from a third pyrazine-2-carboxylate ligand, and by the O atom of a water molecule (Fig. 1). The Ni–N bond lengths range from 2.083 (3) to 2.125 (3) Å and are slightly longer than the Ni–O bond lengths, which range from 2.026 (3) to 2.061 (3) Å.

The bridging of adjacent Ni^{II} atoms by one of the pyrazine-2-carboxylate ligands through its two N atoms leads to a polymeric structure, with zigzag chains extending parallel to

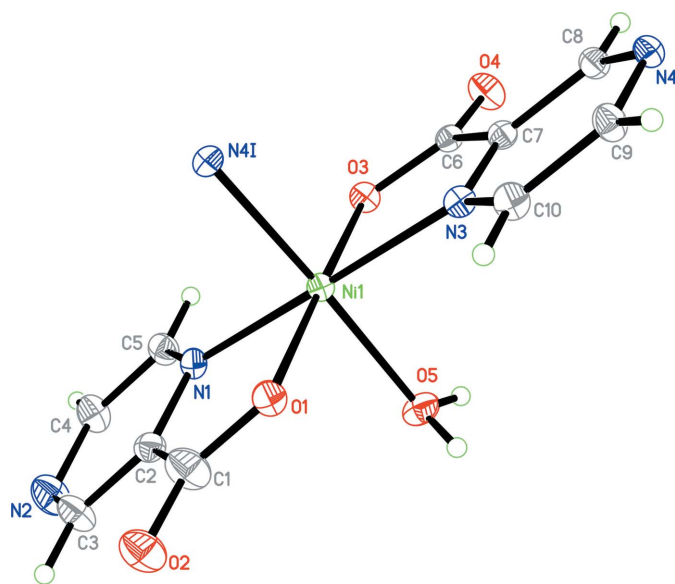


Figure 1
The asymmetric unit of (I), expanded to show the complete coordination of Ni, drawn with 30% probability displacement ellipsoids. [Symmetry code: (I) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$].

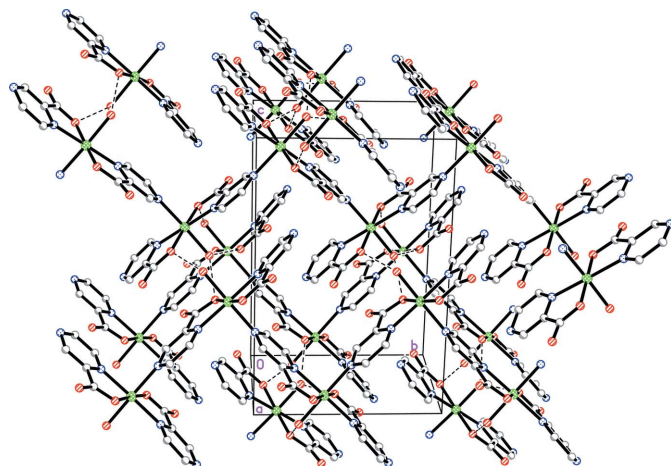


Figure 2
Packing diagram of (I). Ni atoms are represented by green cross-hatched spheres, N atoms by blue dotted spheres, O atoms by red hatched spheres and C atoms by grey shaded spheres. H atoms have been omitted for clarity.

the *b* axis. Medium-strong hydrogen bonding between the water molecules and carboxylate O atoms (Table 2) additionally stabilizes the structure, forming a three-dimensional framework with pores (Fig. 2).

Experimental

A mixture of nickel(II) chloride (0.5 mmol), potassium hydroxide (0.5 mmol) and pyrazine-2-carboxylic acid (0.5 mmol) in H₂O (30 ml) was stirred for 1 h and then filtered. The filtrate was evaporated slowly in air. Green block-shaped crystals of (I) were obtained in a yield of 38%. Analysis calculated for C₁₀H₈N₄O₅Ni: C 37.20, H 2.50, N 17.35, Ni 18.18%; found: C 37.18, H 2.46, N 17.36, Ni 18.33%.

Crystal data

[Ni(C₅H₃N₂O₂)₂(H₂O)]
M_r = 322.91
 Orthorhombic, *P*2₁2₁2₁
a = 7.8001 (2) Å
b = 9.8818 (12) Å
c = 14.9112 (6) Å
V = 1149.34 (15) Å³

Z = 4
D_x = 1.866 Mg m⁻³
 Mo *K*α radiation
μ = 1.72 mm⁻¹
T = 298 (2) K
 Block, green
 0.19 × 0.17 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and *ω* scans
 Absorption correction: none
 6209 measured reflections

2140 independent reflections
 1969 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.027
*θ*_{max} = 25.5°

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.034
wR(*F*²) = 0.085
S = 1.00
 2140 reflections
 175 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2 + 1.048P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δσ)_{max} = 0.001
 Δρ_{max} = 1.05 e Å⁻³
 Δρ_{min} = -0.36 e Å⁻³
 Absolute structure: Flack (1983),
 with 987 Friedel pairs
 Flack parameter: 0.462 (18)

Table 1

Selected bond lengths (Å).

Ni1—O3	2.026 (3)	Ni1—N1	2.083 (3)
Ni1—O1	2.032 (3)	Ni1—N3	2.092 (3)
Ni1—O5	2.061 (3)	Ni1—N4 ⁱ	2.125 (3)

Symmetry code: (i) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$.

Table 2

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>
O5—H2...O3 ⁱⁱ	0.85	2.06	2.763 (4)	140
O5—H1...O1 ⁱⁱⁱ	0.85	1.85	2.695 (4)	173

Symmetry codes: (ii) $x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (iii) $x - \frac{1}{2}, -y + \frac{3}{2}, -z + 1$.

The structure was refined from an inversion-twinned crystal with a twin ratio close to 1:1. The H atoms of the water molecule were located in a difference density map and refined with distance restraints of H...H = 1.38 (2) Å and O—H = 0.88 (2) Å, and with a fixed *U*_{iso}(H) = 0.80 Å². All other H atoms were placed in calculated positions, with C—H = 0.93 Å and with *U*_{iso}(H) = 1.2*U*_{eq}(C). The highest peak is located 1.11 Å from atom O1.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

References

- Bruker (1998). *SMART*. Version 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.
 Bruker (1999). *SAINT* (Version 6.12) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
 Chung, L., Rajan, K. S., Merdinger, E. & Crez, N. (1971). *Biophys. J.* **11**, 469–475.

- Church, B. S. & Halvorson, H. (1959). *Nature*, **183**, 124–125.
- Flack, H. D. (1983). *Acta Cryst. A* **39**, 876–881.
- Kim, Y., Lee, E. & Jung, D. Y. (2001). *Chem. Mater.* **13**, 2684–2699.
- Okabe, N. & Oya, N. (2000). *Acta Cryst. C* **56**, 1416–1417.
- Pocker, Y. & Fong, C. T. O. (1980). *Biochemistry*, **19**, 2045–2049.
- Scapin, G., Reddy, S. G., Zheng, R. & Blanchard, J. S. (1997). *Biochemistry*, **36**, 15081–15088.
- Serre, C., Marrot, J. & Ferey, G. (2005). *Inorg. Chem.* **44**, 654–658.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.