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Key indicators

Single-crystal X-ray study

T = 293 K

Mean $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$

R factor = 0.048

wR factor = 0.123

Data-to-parameter ratio = 15.1

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Poly[[diaquanickel(II)]- μ -(4-pyridylsulfanyl)-
acetato-nickel(II)-tri- μ -(4-pyridylsulfanyl)acetato]

In the linear-chain title compound, $[\text{Ni}_2(\text{C}_7\text{H}_6\text{NO}_2\text{S})_4(\text{H}_2\text{O})_2]_n$, the two Ni atoms occupy inversion centers: one is covalently bonded to two monodentate carboxylate anions, and coordinated by two water molecules and by the pyridyl N atoms of another two carboxylate anions; the second Ni atom is chelated by two carboxylate anions and is also coordinated by the pyridyl N atoms of two carboxylate anions. Both Ni atoms are six-coordinate in distorted octahedral geometries.

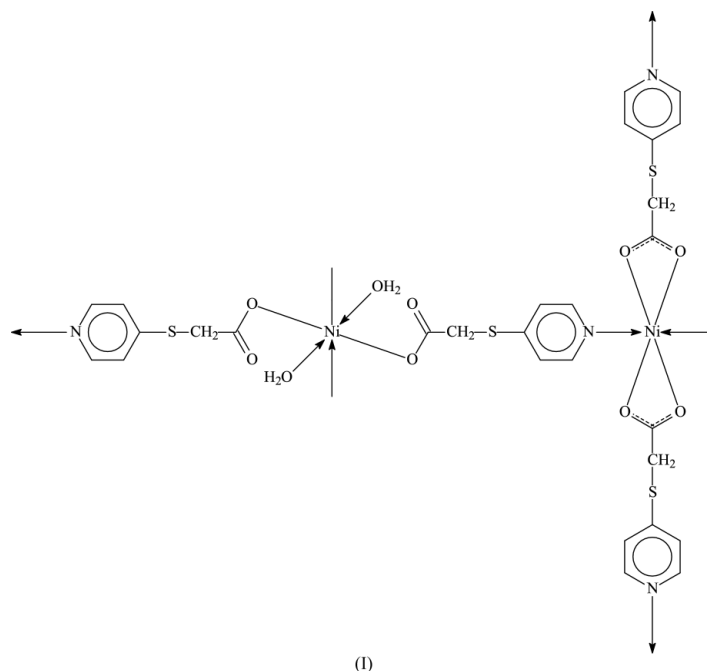
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Comment

With a metal salt–acid stoichiometry of 1:1, the reaction of nickel acetate and pyridyl-4-thiolyacetic acid under hydrothermal conditions yields aquabis(pyridyl-4-thiolyacetato)-nickel, $[\text{Ni}(\text{C}_7\text{H}_6\text{NO}_2\text{S})_2(\text{H}_2\text{O})]_n$ (Huang *et al.*, 2004). With a 1:2 stoichiometry, the compound has an identical empirical formula, but the compound is $[\text{Ni}(\text{C}_7\text{H}_6\text{NO}_2\text{S})_2(\text{H}_2\text{O})_2]_n$ [$\text{Ni}(\text{C}_7\text{H}_6\text{NO}_2\text{S})_2$], (I) (Fig. 1).



The two six-coordinate Ni atoms occupy inversion centers in distorted octahedral geometries. One of them is covalently bonded to two monodentate carboxylate anions; this Ni atom is also coordinated by two water molecules and by the pyridyl N atoms of another two carboxylate anions. The other Ni atom is chelated by two carboxylate anions and is also coordinated by the pyridyl N atoms of two carboxylate anions (Fig. 1). The

bridging behavior of the two carboxylate anions gives rise to a linear-chain structure.

Experimental

Nickel acetate (50 mg, 0.4 mmol), 4-pyridylthioacetic acid (68 mg, 0.4 mmol) and sodium hydroxide (16 mg, 0.4 mmol) were dissolved in a water–ethanol (12:5 v/v) mixture (17 ml). The solution was placed in a Teflon-lined stainless-steel bomb (23 ml). The bomb was heated at 393 K for 12 h and then cooled to room temperature. CHN elemental analysis on the pale-blue platelets found (calculated) for C₁₄H₁₄N₂NiO₅S₂ (%): C 40.47 (40.70), H 3.41 (3.42), N 6.34% (6.78)%. IR (KBr): 3427, 2966, 2921, 1598, 1577, 1562, 1486, 1430, 1373, 1218, 1150, 1115, 1064, 1011, 898, 817, 803, 723, 692, 587, 503 cm⁻¹.

Crystal data

[Ni₂(C₇H₆NO₂S)₄(H₂O)₂]
M_r = 826.20
 Monoclinic, *P*2₁/*a*
a = 15.775 (1) Å
b = 5.7314 (4) Å
c = 16.950 (1) Å
 β = 97.726 (1)°
V = 1518.6 (2) Å³
Z = 2
D_x = 1.807 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 3044 reflections
 θ = 2.4–28.3°
 μ = 1.58 mm⁻¹
T = 293 (2) K
 Plate, pale blue
 0.19 × 0.13 × 0.03 mm

Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
T_{min} = 0.791, *T_{max}* = 0.954
 8645 measured reflections
 3436 independent reflections
 3052 reflections with *I* > 2σ(*I*)
R_{int} = 0.029
 θ_{max} = 27.5°
h = -20 → 19
k = -7 → 5
l = -21 → 22

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.048
wR(*F*²) = 0.123
S = 1.13
 3436 reflections
 228 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.8297P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} = 0.001
 Δρ_{max} = 0.69 e Å⁻³
 Δρ_{min} = -0.44 e Å⁻³

Table 1 Selected geometric parameters (Å, °).

Ni1–N2	2.035 (2)	Ni2–N1	2.106 (2)
Ni1–O1	2.086 (2)	Ni2–O3	2.091 (2)
Ni1–O2	2.138 (2)	Ni2–O1w	2.057 (2)
N2–Ni1–O1	87.08 (9)	N1–Ni2–O3	89.37 (9)
N2–Ni1–O1 ⁱ	92.92 (9)	N1–Ni2–O3 ⁱⁱ	90.63 (9)
N2–Ni1–O2	88.52 (9)	N1–Ni2–O1w	85.00 (9)
N2–Ni1–O2 ⁱ	91.48 (9)	N1–Ni2–O1w ⁱⁱ	95.00 (9)
O1–Ni1–O2	62.27 (8)	O3–Ni2–O1w	85.81 (9)
O1–Ni1–O2 ⁱ	117.73 (8)	O3–Ni2–O1w ⁱⁱ	94.19 (9)

Symmetry codes: (i) 1 - *x*, 1 - *y*, 1 - *z*; (ii) 1 - *x*, 1 - *y*, 2 - *z*.

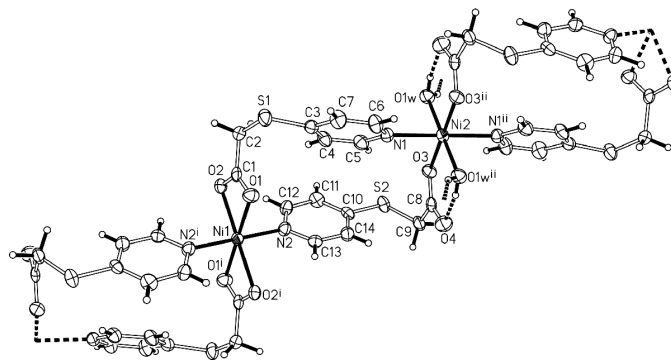


Figure 1 ORTEPII (Johnson, 1976) plot of (I) with displacement ellipsoids at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. [Symmetry codes: (i) 1 - *x*, 1 - *y*, 1 - *z*; (ii) 1 - *x*, 1 - *y*, 2 - *z*.]

Table 2 Hydrogen-bonding 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–H1w2...O3 ⁱⁱⁱ	0.85 (1)	2.15 (2)	2.943 (3)	155 (4)
O1w–H1w1...O4 ⁱⁱ	0.85 (1)	1.82 (2)	2.648 (3)	163 (4)

Symmetry codes: (ii) 1 - *x*, 1 - *y*, 2 - *z*; (iii) 1 - *x*, 2 - *y*, 2 - *z*.

The water H atoms were located in a difference map and refined with distance restraints of O–H = 0.85 (1) Å and H...H = 1.39 (1) Å. The aromatic (C–H = 0.93 Å) and aliphatic (C–H = 0.97 Å) H atoms were placed at calculated positions and refined in the riding-model approximation, with *U*_{iso}(H) = 1.2*U*_{eq}(C).

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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