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catena-Poly[[aquanickel(II)]-di-μ-(4-pyridylsulfanyl)acetato-κ^6N:*O*,*O*;*O*,*O*′:*N*]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.095
Data-to-parameter ratio = 15.6

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

The water-coordinated Ni atom in the title compound, $[Ni(C_7H_6NO_2S)_2(H_2O)]_n$, is covalently bonded to two carboxylate groups (one binding in a monodentate mode and the other in a chelating mode); it is also linked to the N atoms of two other carboxylate anions in an octahedral environment. The compound adopts a linear chain architecture; adjacent chains are linked into layers by hydrogen bonds.

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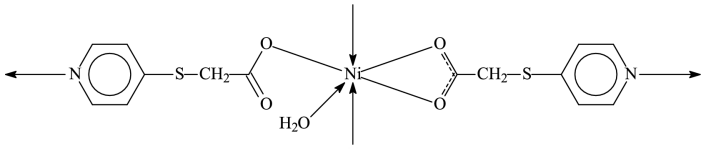
Comment

A number of compounds resulting from the reaction of pyridyl-4-thiolylacetic acid with metal salts have been crystallographically authenticated; some of these are neutral complexes whereas others are zwitterions (Qin *et al.*, 2004; Zhang *et al.*, 2004*a*,*b*).



(I)

Tetraaquabis(pyridyl-4-thiolylacetato)nickel(II), which exists as a zwitterion, was synthesized hydrothermally in a nearly neutral aqueous solvent system; the reaction when carried out at a lower temperature and for a shorter time gave the title polymeric compound *catena*-poly[[aquanickel(II)]-di-μ-(4-pyridylsulfanyl)acetato], (I) (Fig. 1), whose Ni atom is instead covalently linked to two carboxylate anions. One of the anions functions as a chelate [bite angle = 60.84 (6)°]; its two O atoms, the water molecule and the O atom of a monodentate carboxylate anion are coplanar; the pyridyl N atoms belonging to two other carboxylate anions lie on opposite sides of the plane, these interactions giving rise to a chain motif (Fig. 2).

Experimental

Nickel acetate (100 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 analyses on the green crystals found (calculated) for $C_{14}H_{14}N_2NiO_5S_2$ (%): C 40.23 (40.70), H 3.42 (3.42), N 6.64 (6.78). IR (KBr): 3385, 2921, 1599, 1579, 1561, 1487, 1430, 1376, 1218, 1147, 1119, 1057, 817, 804, 724, 701, 589, 503 cm^{-1}.

Crystal data

$[Ni(C_7H_6NO_2S)_2(H_2O)]$
M_r = 413.10
Triclinic, $P\overline{1}$
a = 8.1693 (4) Å
b = 10.3430 (5) Å
c = 10.6876 (5) Å
α = 67.371 (1)°
β = 73.176 (1)°
γ = 86.825 (1)°
V = 796.25 (7) Å^3
Z = 2
D_x = 1.723 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5217 reflections
θ = 2.8–26.3°
μ = 1.51 mm^{-1}
T = 293 (2) K
Prism, green
0.13 × 0.12 × 0.10 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.665, T_{max} = 0.864
6789 measured reflections
3511 independent reflections
3266 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 27.5°
$h = -10 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.095
S = 1.06
3511 reflections
225 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.2563P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O3	2.023 (2)	Ni1—O1*w*	2.049 (2)
Ni1—O1	2.094 (2)	Ni1—N1^{i}	2.099 (2)
Ni1—O2	2.210 (2)	Ni1—N2^{ii}	2.094 (2)
O1—Ni1—O2	60.84 (6)	O2—Ni1—N2^{ii}	92.02 (7)
O1—Ni1—O3	166.10 (6)	O3—Ni1—N1^{i}	88.82 (7)
O1—Ni1—O1*w*	98.41 (6)	O3—Ni1—N2^{ii}	90.56 (7)
O1—Ni1—N1^{i}	88.55 (6)	O3—Ni1—O1*w*	95.20 (7)
O1—Ni1—N2^{ii}	91.65 (6)	O1*w*—Ni1—N1^{i}	89.29 (7)
O2—Ni1—O3	105.37 (6)	O1*w*—Ni1—N2^{ii}	92.43 (7)
O2—Ni1—O1*w*	158.89 (7)	N1^{i}—Ni1—N2^{ii}	178.21 (7)
O2—Ni1—N1^{i}	86.52 (6)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*w*—H1*w*2···O1^{iii}	0.84 (1)	1.88 (1)	2.722 (2)	176 (3)
O1*w*—H1*w*1···O4	0.85 (1)	1.83 (2)	2.633 (2)	158 (3)

Symmetry code: (iii) $1-x, 1-y, 2-z$.

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 using the riding-model approximation, with U_{iso}= 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

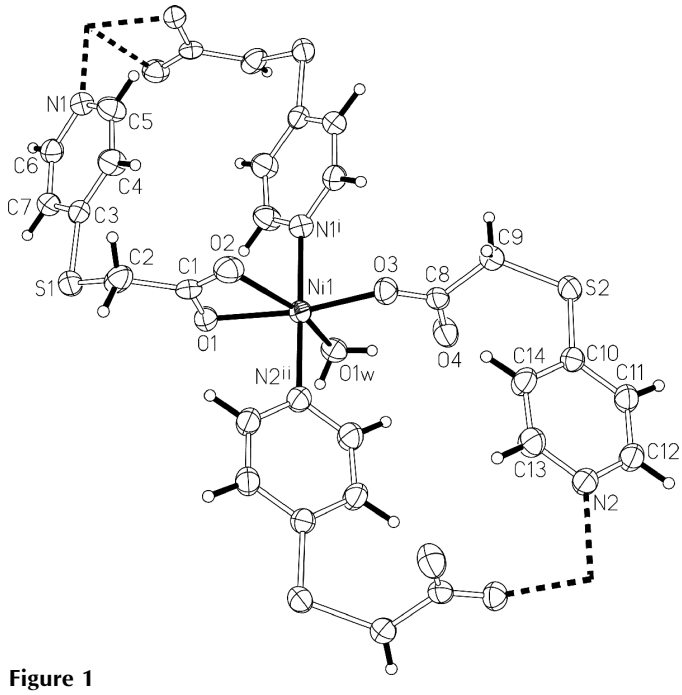


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii. [Symmetry codes: (i) $1-x, 2-y, 2-z$; (ii) $1-x, 1-y, 1-z$.]

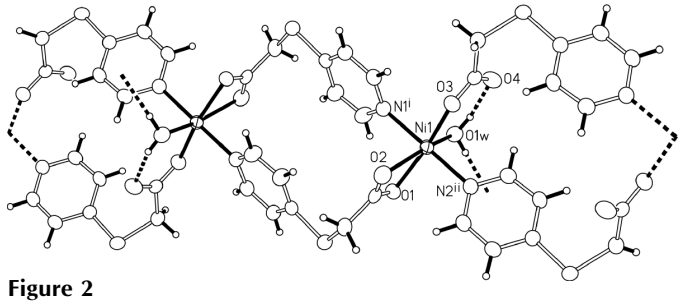


Figure 2
*ORTEP*II (Johnson, 1976) plot of the chain structure of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii. [Symmetry codesas for Fig. 1.]

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