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Tetraaquabis(4-pyridylthioacetato)nickel(II)

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The Ni atom in the zwitterionic title compound, $[Ni(C_7H_6NO_2S)_2(H_2O)_4]$, lies on a centre of symmetry. It is linked to the pyridyl N atom of two anionic groups and to four water molecules in an octahedral environment. The zwitterions are connected by hydrogen bonds into a three-dimensional network structure.

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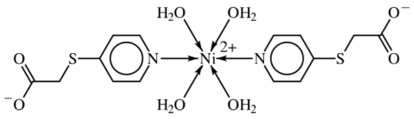
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.026
wR factor = 0.072
Data-to-parameter ratio = 12.0

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

Comment

The reaction of copper nitrate and the ammonium salt of 4-pyridylthioacetic acid yields $[Cu(C_7H_6NO_2S)_2(H_2O)_2(NH_3)_2]$, which is zwitterionic, with the the 4-pyridylthioacetate anion bonding through the pyridyl N atom. The amine donor in the molecule arises from the slight excess of ammonium hydroxide that was used to neutralize the carboxylic acid (Huang *et al.*, 2004). A similar reaction with a nickel salt, but with sodium hydroxide in place of ammonium hydroxide, afforded the corresponding tetraaquanickel complex, *viz.* the title complex, (I) (Fig. 1), which also exists as a zwitterion. The octahedrally coordinated Ni atom lies on a centre of symmetry. Hydrogen bonds link the zwitterions into a three-dimensional network structure. Bond dimensions involving Ni are similar to those found in the zwitterionic tetraaquanicotinatonickel (Batten & Harris, 2001*b*) and tetraaquaisonicotinatonickel (Batten & Harris, 2001*a*; Min *et al.*, 2001; Ng, 2003) complexes, which also feature extensive hydrogen-bonding interactions.



(I)

Experimental

A mixture of nickel sulfate hexahydrate (0.26 g, 1.0 mmol), 4-pyridylthioacetic acid (0.25 g, 1.5 mmol) and water (7 ml) was treated with drops of 2 N sodium hydroxide to give a pH of approximately 7. The solution was transferred into a 15 ml Teflon-lined stainless-steel bomb, which was then heated at 433 K for 96 h. After cooling to room temperature, blue crystals separated from the solution in about 50% yield. CHN analysis: C 35.94, H 4.36, N 5.96, S 13.64%; calculated for $C_{14}H_{20}N_2NiO_8S_2$: C 36.00, H 4.32, N 6.00, S 13.73%.

Crystal data

$[Ni(C_7H_6NO_2S)_2(H_2O)_4]$
M_r = 467.15
Monoclinic, $P2_1/a$
a = 7.4924 (5) Å
b = 10.4589 (7) Å
c = 12.1369 (8) Å
β = 107.393 (1)°
V = 907.6 (1) Å^3
Z = 2

D_x = 1.709 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3212 reflections
θ = 2.6–26.9°
μ = 1.35 mm^{-1}
T = 298 (2) K
Plate, blue
0.35 × 0.19 × 0.09 mm

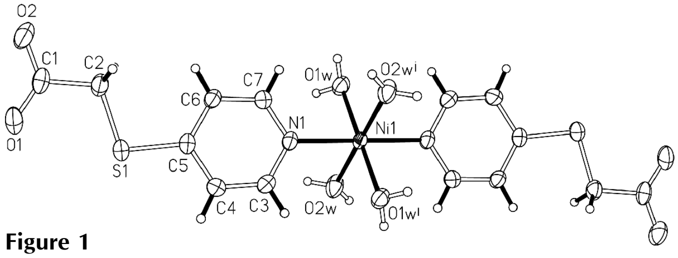


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with ellipsoids drawn at the 50% probability level. The symmetry code is given in Table 1.

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.753$, $T_{\max} = 0.889$
5157 measured reflections
1960 independent reflections
1813 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.015$
$\theta_{\max} = 27.0°$
$h = -8 \rightarrow 9$
$k = -13 \rightarrow 11$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.072$
$S = 1.04$
1960 reflections
164 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 0.1843P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.37$ e Å^{-3}
$\Delta\rho_{\min} = -0.17$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1*w*	2.071 (1)	Ni1—N1	2.106 (1)
Ni1—O2*w*	2.044 (1)		
O1*w*—Ni1—O1*w*^{i}	180	O2*w*—Ni1—O2*w*^{i}	180
O1*w*—Ni1—O2*w*	89.1 (1)	O2*w*—Ni1—N1	87.5 (1)
O1*w*—Ni1—O2*w*^{i}	90.9 (1)	O2*w*—Ni1—N1^{i}	92.5 (1)
O1*w*—Ni1—N1	91.0 (1)	N1—Ni1—N1^{i}	180
O1*w*—Ni1—N1^{i}	89.0 (1)		

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

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

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
O1*w*—H1*w*1$\cdots$O1^{ii}	0.84 (1)	1.93 (1)	2.759 (2)	168 (3)
O1*w*—H1*w*2$\cdots$O1^{iii}	0.84 (1)	2.02 (1)	2.842 (2)	165 (2)
O2*w*—H2*w*1$\cdots$O2^{iv}	0.83 (1)	1.92 (1)	2.744 (2)	168 (2)
O2*w*—H2*w*2$\cdots$O2^{ii}	0.84 (1)	1.89 (1)	2.729 (2)	177 (3)

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

The crystal used in the measurements diffracted sufficiently strongly for all H atoms to be located and refined with distance restraints [O—H = 0.85 (1) Å and C—H = 0.95 (1) Å].

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); method used to solve structure: difference Fourier, with Ni at ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$); 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.

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