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Key indicators

Single-crystal X-ray study
 T = 298 K
 Mean $\sigma(C-C)$ = 0.003 Å
 H-atom completeness 98%
 Disorder in solvent or counterion
 R factor = 0.032
 wR factor = 0.083
 Data-to-parameter ratio = 15.9

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

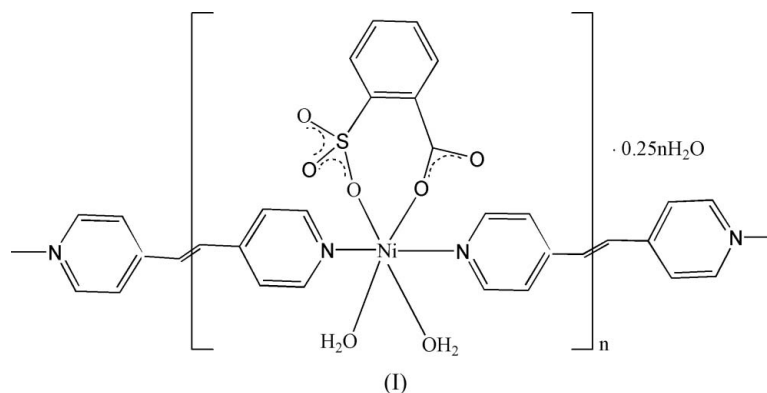
catena-Poly[[[diaqua(2-sulfonatobenzoato)nickel(II)]-
 μ -1,2-di-4-pyridylethylene] 0.25-hydrate]

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In the title compound, $\{[Ni(C_7H_4O_5S)(C_{12}H_{10}N_2)(H_2O)_2] \cdot 0.25H_2O\}_n$, the Ni^{II} atom has a distorted octahedral environment formed by two N and four O atoms. The 1,2-di-4-pyridylethylene ligands, which lie on inversion centers, function as μ_2 -bridging ligands to form a linear chain. The 2-sulfonatobenzoate ligands protrude alternately on both sides of the linear chain and chelate to the Ni^{II} atoms through one carboxylate O atom and one sulfonate O atom.

Comment

The sulfonate group can exhibit very different coordination behavior compared to the carboxylate group in the constructions of metal-organic coordination polymers (Fan *et al.*, 2004; Wang *et al.*, 2004; Zheng *et al.*, 2003). Numerous benzene-1,2-dicarboxylate complexes have been extensively studied (Thirumurugan & Natarajan, 2004; Yao *et al.*, 2002). However, complexes with 2-sulfonatobenzoate (*o*-sb), a ligand with a combination of sulfonate and carboxylate groups, are rather limited (Li & Yang, 2004; Su *et al.*, 2005). We report here a one-dimensional coordination polymer with the *o*-sb ligand, $\{[Ni(o-sb)(bpe)(H_2O)_2] \cdot 0.25H_2O\}$ (bpe is 1,2-di-4-pyridylethylene), (I).



The Ni^{II} atom in (I) has an octahedral geometry defined by two aqua O atoms, two O atoms from one *o*-sb ligand and two N atoms from two bpe ligands (Fig. 1). The Ni1—O bond lengths are in the range 2.0567 (13)–2.1358 (14) Å. The *trans* angles of the octahedron are 172.19 (5), 173.65 (6) and 177.77 (5)°, and the other angles are in the range 86.21 (6)–97.74 (6)° (Table 1). The *o*-sb ligand chelates to the Ni^{II} center to form a six-membered ring. The dihedral angle between the planes of the *o*-sb ring and its carboxylate group is 12.6 (3)°. The C1—O1 bond length [1.265 (2) Å] is longer than the C1—O2 distance [1.247 (2) Å], indicating more keto character in the latter. The two crystallographically independent centro-

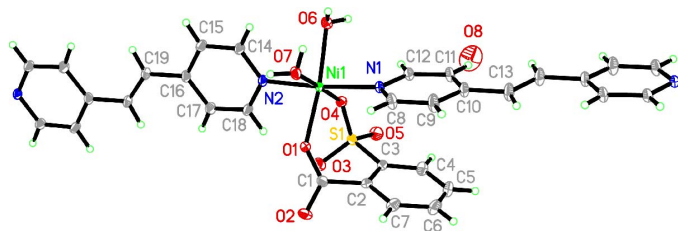


Figure 1

The coordination environment of atom Ni1 in (I), showing the atom numbering and displacement ellipsoids at the 30% probability level. The unlabelled atoms of the left- and right-hand bridging ligands are related to the labelled atoms by $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$ and $\frac{1}{2} + x, \frac{1}{2} + y, 2 + z$, respectively.

symmetric bpe ligands function as μ_2 -bridging ligands, forming a linear chain. The *o*-sb ligands protrude on both sides of the linear chain (Fig. 2).

In the crystal structure, there are three intermolecular hydrogen bonds between the two coordinated water molecules and two carboxylate O atoms. The coordinated water atom O6 forms a hydrogen bond with atom O5 of an adjacent chain (Table 2). A three-dimensional network structure is thus formed by these hydrogen-bond interactions.

Experimental

Nickel(II) acetate tetrahydrate (0.5 mmol), 2-sulfobenzoic acid (0.5 mmol) and 1,2-di-4-pyridylethylene (1.0 mmol) were placed in a 30 ml Teflon-lined stainless steel Parr bomb together with water (20 ml). The bomb was heated at 423 K for 6 d. The bomb was cooled slowly to room temperature to furnish green crystals.

Crystal data

$[\text{Ni}(\text{C}_7\text{H}_4\text{O}_5\text{S})(\text{C}_{12}\text{H}_{10}\text{N}_2)(\text{H}_2\text{O})_2] \cdot 0.25\text{H}_2\text{O}$	$D_x = 1.572 \text{ Mg m}^{-3}$
$M_r = 481.63$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 6367 reflections
$a = 17.1636 (9) \text{ \AA}$	$\theta = 2.4\text{--}28.2^\circ$
$b = 16.5180 (9) \text{ \AA}$	$\mu = 1.10 \text{ mm}^{-1}$
$c = 14.6151 (8) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\beta = 100.798 (1)^\circ$	Prism, green
$V = 4070.1 (4) \text{ \AA}^3$	$0.35 \times 0.27 \times 0.23 \text{ mm}$
$Z = 8$	

Data collection

Bruker SMART CCD area-detector diffractometer	4429 independent reflections
φ and ω scans	4072 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$R_{\text{int}} = 0.020$
$T_{\text{min}} = 0.699, T_{\text{max}} = 0.786$	$\theta_{\text{max}} = 27.0^\circ$
12199 measured reflections	$h = -21 \rightarrow 17$
	$k = -21 \rightarrow 17$
	$l = -18 \rightarrow 18$

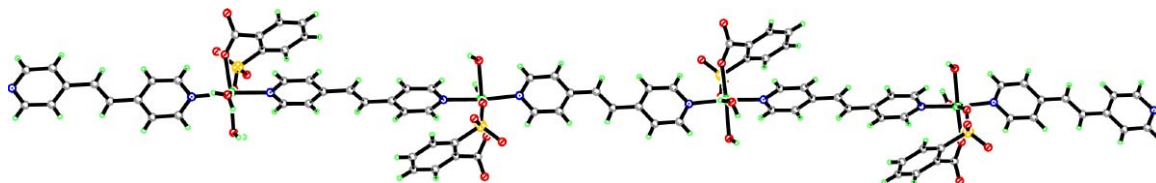


Figure 2

Illustration of a linear chain in (I).

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.083$
 $S = 1.03$
 4429 reflections
 278 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 5.4805P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.002$
 $\Delta\rho_{\text{max}} = 0.63 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.36 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters ($\text{\AA}, ^\circ$).

Ni1—O1	2.0567 (13)	Ni1—N1	2.0963 (15)
Ni1—O7	2.0690 (13)	Ni1—O6	2.1358 (14)
Ni1—O4	2.0812 (13)	O1—C1	1.265 (2)
Ni1—N2	2.0856 (15)	O2—C1	1.247 (2)
O1—Ni1—O7	86.86 (6)	O4—Ni1—N1	88.43 (6)
O1—Ni1—O4	90.97 (5)	N2—Ni1—N1	173.65 (6)
O7—Ni1—O4	177.77 (5)	O1—Ni1—O6	172.19 (5)
O1—Ni1—N2	88.13 (6)	O7—Ni1—O6	86.31 (6)
O7—Ni1—N2	91.39 (6)	O4—Ni1—O6	95.89 (5)
O4—Ni1—N2	89.06 (6)	N2—Ni1—O6	88.25 (6)
O1—Ni1—N1	97.74 (6)	N1—Ni1—O6	86.21 (6)
O7—Ni1—N1	91.34 (6)		

Table 2

Hydrogen-bonding geometry ($\text{\AA}, ^\circ$).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
O7—H7B \cdots O1 ⁱ	0.81	2.02	2.8273 (18)	173
O7—H7A \cdots O2 ⁱⁱ	0.82	1.90	2.720 (2)	175
O6—H6B \cdots O2 ⁱⁱ	0.81	2.03	2.827 (2)	168
O6—H6A \cdots O5 ⁱⁱⁱ	0.82	2.02	2.757 (2)	149

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

H atoms attached to C atoms were included in the refinement at calculated positions in the riding-model approximation [$C\text{---}H = 0.93 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$]. The water H atoms were located and refined with distance restraints $O\text{---}H = 0.82 (1) \text{ \AA}$ and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. At this stage, the maximum difference density of 4.59 \AA^{-3} indicated the presence of a possible atom site. This peak was found near atom H1, at a hydrogen-bonding distance of 2.85 \AA . Attempts to refine this peak as a water O atom (O8) with full occupancy resulted in a high U_{iso} value, and hence it was refined with partial occupancy. The occupancy of O8 was initially refined to 0.26 (1) and later fixed at 0.25. Positioning of H atoms attached to O8 was not possible.

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: XP (Bruker, 2002); software used to prepare material for publication: SHELXTL (Bruker, 2002).

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