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catena-Poly[[[aqua(2,2′-bipyridine-*N*,*N*′)-nickel(II)]-μ-3,5-dinitrosalicylato-κ^3*O*,*O*′:*O*″] 0.2-hydrate]

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In the title complex, $\{[\mathrm{Ni(C_7H_2N_2O_7)(C_{10}H_8N_2)(H_2O)}]\cdot 0.2\mathrm{H_2O}\}_n$, the Ni$^{\mathrm{II}}$ atom is coordinated by three O atoms from two symmetry-related 3,5-dinitrosalicylate ligands, two N atoms from one 2,2′-bipyridine and one water molecule, and its environment displays a distorted octahedral geometry. The short face-to-face distances between parallel 2,2′-bipyridine planes of neighbouring complexes and neighbouring one-dimensional chains indicate π–π stacking. The packing is further influenced by inter- and intramolecular hydrogen-bond interactions.

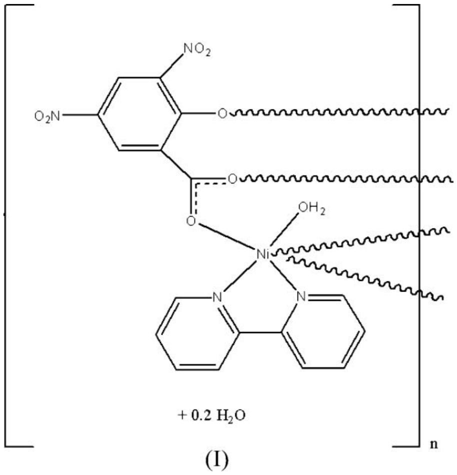
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
H-atom completeness 97%
Disorder in solvent or counterion
R factor = 0.035
wR factor = 0.099
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.

Comment

We have recently been interested in the nature of π–π stacking, as it plays an important role in some biological processes (Deisenhofer & Michel, 1989). A series of metal complexes incorporating different aromatic ligands has been prepared and their crystal structures provide useful information on π–π stacking (Wu *et al.*, 2003; Pan & Xu, 2004; Li *et al.*, 2005). As part of our ongoing investigations, the title complex, (I), incorporating 3,5-dinitrosalicylate and 2,2′-bipyridine, has been prepared.



(I)

The Ni$^{\mathrm{II}}$ centre in (I) presents a distorted octahedral geometry (Fig. 1) defined by three O atoms from two symmetry-related 3,5-dinitrosalicylate ligands, two N atoms from one 2,2′-bipyridine and one water molecule. A disordered water solvent molecule (occupancy 0.20) completes the structure and O6 showed a larger than average displacement parameter, probably implying some kind of disorder. Selected parameters of the Ni$^{\mathrm{II}}$ coordination polyhedron are given in Table 1.

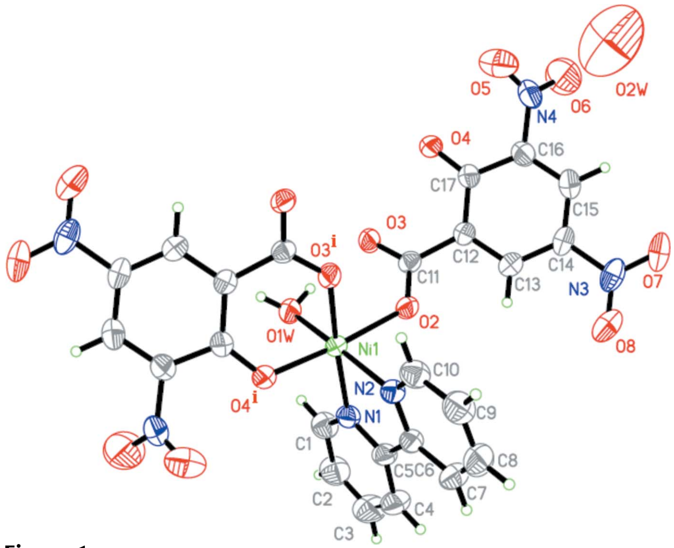


Figure 1

Part of the polymeric chain structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code as in Table 1.

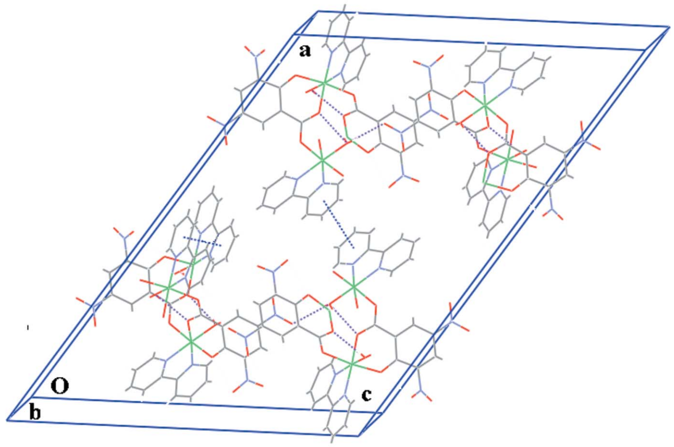


Figure 2

A packing view of (I), showing the inter- and intramolecular hydrogen bonds and the π–π interactions as broken lines. H atoms and solvent water molecules have been omitted for clarity.

The polymeric chains are further linked by weak O—H···O hydrogen bonds (Table 2) and π–π stacking interactions between the N2/C6–C10 and N1a/C1a–C5a rings [symmetry code: (a) x, $1 + y$, z; face-to-face distance = 3.66 (1) Å] between neighbouring complexes (Fig. 2). Meanwhile, another set of O—H···O interactions (Table 2) and π–π bonds between the N1b/C1b–C5b (b = 1.5-x, 0.5+y, 1.5-z) and N2c/C6c–C10c rings [symmetry codes: (b) $\frac{3}{2} - x$, $\frac{1}{2} + y$, $\frac{3}{2} - z$; (c) $-\frac{1}{2} + x$, $\frac{1}{2} - y$, $-\frac{11}{22} + x$; face-to-face distance = 3.75 (1) Å] serves to assemble the three-dimensional structure (Fig. 2).

Experimental

The title complex was prepared by the addition of stoichiometric amounts of nickel(II) chloride (20 mmol) and 2,2′-bipyridine (20 mmol) to a hot aqueous solution (30 ml) of 3,5-dinitrosalicylic acid (20 mmol). The pH was then adjusted to 7.0–8.0 with NaOH (30 mmol). The resulting solution was filtered, and cyan single crystals of (I) were obtained at room temperature over several days.

Crystal data

$[Ni(C_7H_2N_2O_7)(C_{10}H_8N_2)(H_2O)]\cdot 0.2H_2O$
$M_r = 462.62$
Monoclinic, $C2/c$
$a = 31.9347\ (14)$ Å
$b = 6.4537\ (3)$ Å
$c = 22.7534\ (11)$ Å
$\beta = 126.278\ (5)°$
$V = 3780.4\ (4)$ Å^3
$Z = 8$
$D_x = 1.613$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.08$ mm^{-1}
$T = 293\ (2)$ K
Block, cyan
0.25 × 0.23 × 0.22 mm

Data collection

Bruker APEXII area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.77$, $T_{max} = 0.79$
28778 measured reflections
4354 independent reflections
3459 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 27.6°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.099$
$S = 1.06$
4354 reflections
280 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 2.1068P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

Table 1

Selected bond lengths (Å).

Ni1—N1	2.0536 (19)	Ni1—O4^i	2.0364 (15)
Ni1—N2	2.0671 (19)	Ni1—O1W	2.0877 (16)
Ni1—O3^i	2.0212 (16)	Ni1—O2	2.1046 (15)

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

Table 2

Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H2W···O7^{ii}	0.81	2.06	2.840 (2)	162
O1W—H1W···O3	0.80	1.90	2.659 (2)	160

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

The occupancy factor of the disordered solvent water molecule (O2W) was refined in the initial stages and then kept fixed in the last cycles of refinement; the corresponding H atoms were excluded from the model. The H atoms of the coordinated water molecule O1W, were located in a difference Fourier map. The remaining H atoms in the aromatic ring were placed in calculated positions, with C—H = 0.93 Å. All H atoms in the structure were allowed to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}$(parent), where $x = 1.2$ for C and 1.5 for O. Atom O6 showed a larger-than-average displacement parameter, probably implying some kind of disorder; no attempt was made to model this.

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

Acta Cryst. (2007). E**63**, m610–m612 Song *et al.* • $[Ni(C_7H_2N_2O_7)(C_{10}H_8N_2)(H_2O)]\cdot 0.2H_2O$ **m611**

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m612 Song *et al.* • [Ni($C_7H_2N_2O_7$)($C_{10}H_8N_2$)(H_2O)]·0.2H_2O *Acta Cryst.* (2007). E**63**, m610–m612