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Aquabis(1,10-phenanthroline)(4,4′-sulfonyldibenzoato)nickel(II) dihydrate

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In the title compound, $[Ni(C_{14}H_8O_6S)(C_{12}H_8N_2)_2(H_2O)]\cdot 2H_2O$, each Ni atom is coordinated by four N atoms [Ni—N = 2.083 (2)–2.096 (3) Å] from two 1,10-phenanthroline ligands and two O atoms [Ni—O = 2.032 (2) and 2.100 (2) Å] from a 4,4′-sulfonyldibenzoate ligand and a water molecule in a distorted octahedral geometry. The crystal structure exhibits intermolecular O—H···O hydrogen bonds and π–π stacking interactions.

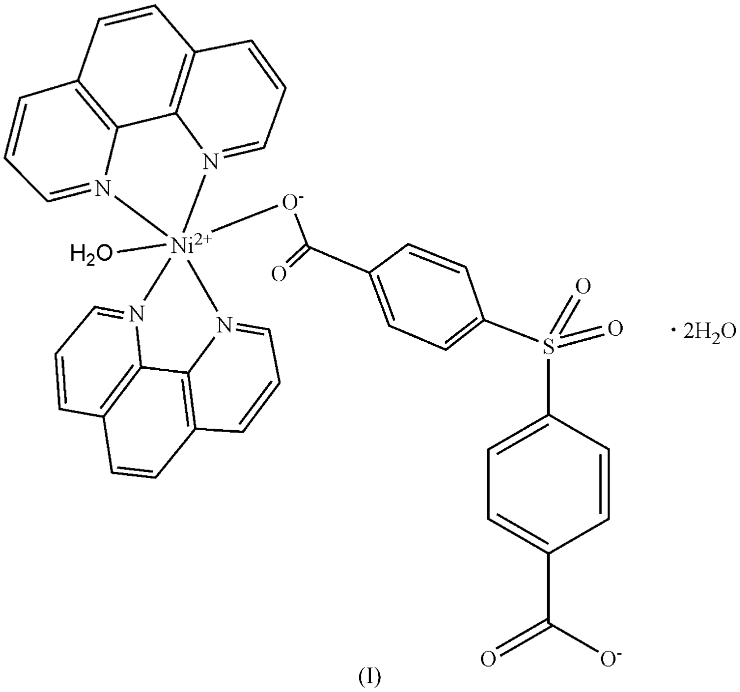
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.056
wR factor = 0.122
Data-to-parameter ratio = 16.1

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

Comment

Recently, the design and synthesis of metal–organic frameworks (MOFs) have led to a large number of coordination polymers (Moulton & Zaworotko, 2001; Kitagawa & Kitaura, 2004; Yaghi *et al.*, 2003). Multidentate *N*- or *O*-donor ligands have been employed extensively as organic spacers in the construction of extended networks (Fujita *et al.*, 1994; Kitagawa & Kondo, 1998; Jung *et al.*, 2000). We have chosen 4,4′-sulfonyldibenzoic acid as a typical V-shaped ligand, which can coordinate the metal ions in bi-, tri- and tetradentate modes, and generate some predicted controlled structural frameworks in variable experimental conditions (Sun *et al.*, 2006; Chen & Lin, 2002; Han *et al.*, 2005). In this paper, we report the synthesis and crystal structure of the title compound, (I).



(I)

In (I) (Fig. 1), each Ni atom is coordinated by four N atoms from two 1,10-phenanthroline ligands and two O atoms from a

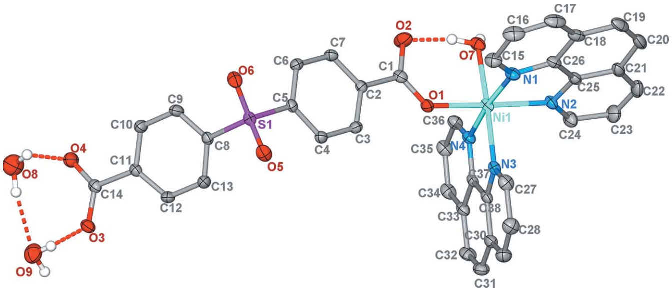


Figure 1
The asymmetric unit of (I), showing the atom numbering and displacement ellipsoids drawn at the 30% probability level. Hydrogen bonds are indicated by dashed lines. The C-bound H atoms have been omitted for clarity.

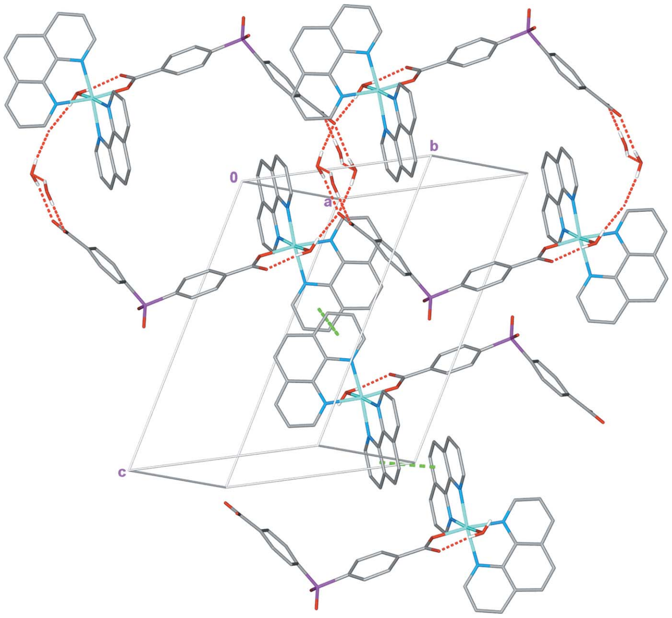


Figure 2
A portion of the crystal packing, showing the intermolecular hydrogen bonds (red) and π–π stacking interactions (green) as dashed lines. H atoms not involved in hydrogen bonds have been omitted.

4,4′-sulfonyldibenzoate ligand and a water molecule in a distorted octahedral geometry (Table 1). The uncoordinated water molecules contribute to the formation of intermolecular O—H⋯O hydrogen bonds (Table 2). The crystal structure (Fig. 2) also exhibits short distances between ring centroids $Cg1\cdots Cg2^{iii}$ [3.521 (2) Å] and $Cg3\cdots Cg3^{iv}$ [3.813 (2) Å] (*Cg*1, *Cg*2 and *Cg*3 are the centroids of rings N4/C33–C37, C30–C33/C37/C38 and N1/C15–C18/C26, respectively), indicating the presence of π–π stacking interactions [symmetry codes: (iii) $1 + x, 1 + y, 1 + z$; (iv) $1 - x, 1 - y, 1 - z$].

Experimental

The title compound, (I), was prepared by the hydrothermal reaction of $Ni(NO_3)_2\cdot 6H_2O$ (0.060 g, 0.20 mmol) and 4,4′-sulfonyldibenzoic acid (0.060 g, 0.20 mmol) in water (8 ml). The reaction was performed in a 23 ml Teflon-lined stainless steel Parr bomb under autogeneous pressure. After heating at 423 K for 3 d and cooling to room temperature at a rate of 5 K h^{-1}, green crystals of (I) were obtained (yield 45%, based on Ni).

Crystal data

$[Ni(C_{14}H_8O_6S)(C_{12}H_8N_2)_2(H_2O)]\cdot 2H_2O$
$M_r = 777.43$
Triclinic, $P\overline{1}$
$a = 8.8457$ (10) Å
$b = 12.4789$ (14) Å
$c = 16.673$ (2) Å
$\alpha = 105.894$ (4)°
$\beta = 105.091$ (4)°
$\gamma = 91.836$ (5)°
$V = 1698.4$ (3) Å^3
$Z = 2$
$D_x = 1.520$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.70$ mm^{-1}
$T = 293$ (2) K
Prism, green
0.35 × 0.25 × 0.10 mm

Data collection

Rigaku Mercury CCD diffractometer
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
$T_{min} = 0.792$, $T_{max} = 0.934$
13188 measured reflections
7689 independent reflections
5663 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.122$
$S = 1.09$
7689 reflections
478 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2 + 0.8893P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	2.032 (2)	Ni1—N3	2.090 (2)
Ni1—N2	2.083 (2)	Ni1—N1	2.096 (2)
Ni1—N4	2.084 (2)	Ni1—O7	2.101 (2)
O1—Ni1—N2	172.65 (10)	N4—Ni1—N1	173.57 (10)
O1—Ni1—N4	93.11 (9)	N3—Ni1—N1	98.44 (9)
N2—Ni1—N4	93.95 (9)	O1—Ni1—O7	91.59 (8)
O1—Ni1—N3	88.40 (9)	N2—Ni1—O7	89.87 (9)
N2—Ni1—N3	90.82 (9)	N4—Ni1—O7	94.64 (9)
N4—Ni1—N3	79.99 (9)	N3—Ni1—O7	174.62 (9)
O1—Ni1—N1	93.08 (9)	N1—Ni1—O7	86.92 (9)
N2—Ni1—N1	79.81 (10)		

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O7—H7*A*⋯O3^{i}	0.85	2.02	2.865 (3)	174
O7—H7*B*⋯O2	0.85	1.82	2.633 (3)	159
O8—H8*B*⋯O9	0.85	2.08	2.897 (4)	160
O8—H8*A*⋯O4	0.85	2.13	2.907 (4)	152
O9—H9*A*⋯O3^{ii}	0.85	2.04	2.879 (3)	171
O9—H9*B*⋯O3	0.85	2.15	2.993 (4)	171

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

The H atoms of water molecules were located in difference Fourier maps. C-bound H atoms were positioned geometrically. All H atoms were refined as riding (C—H = 0.93 Å and O—H = 0.85 Å), with $U_{iso}(H) = 1.2U_{eq}(C,O)$.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve

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structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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