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Tetraaqua(2,2′-bipyridine)nickel(II) terephthalate

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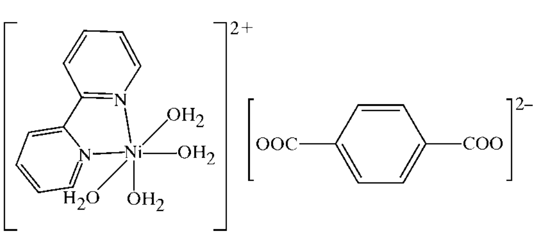
The reaction of nickel(II) nitrate with terephthalic acid and 2,2′-bipyridine in dimethylformamide solution gives the title complex, $[Ni(C_{10}H_8N_2)(H_2O)_4](C_8H_4O_4)$. The Ni^{II} ion is octahedrally coordinated to one 2,2′-bipyridine and four water molecules and does not coordinate to the terephthalate anion. Hydrogen bonds between the terephthalate anions and the $[Ni(2,2'\text{-bipy})(H_2O)_4]^{2+}$ cations produce a two-dimensional hydrogen-bonding architecture with double sheets.

Comment

In recent years, significant research effort has been focused on coordination polymers, due to their potential applications in catalysis, ion exchange and gas adsorption (Eddaoudi *et al.*, 2002; Moulton & Zaworotko, 2001); popular bridging ligands in this field are terephthalic acid (H_2ta) and 4,4′-bipyridine, and their derivatives (Eddaoudi *et al.*, 2001). Numerous complexes with the ta^{2-} ligand have been extensively studied, while new complexes are constantly being synthesized. Although the ta^{2-} ligand has many coordination modes, reports of complexes in which the terephthalate anion is used as a synthon to generate supramolecular networks are still relatively rare (Allen *et al.*, 1999; Burrows *et al.*, 1996, 1997). We report here an example of ta^{2-} as a hydrogen-bonding linker in the presence of *N*-donor ligands. The title compound, (I), consists of an $[Ni(2,2'\text{-bipy})(H_2O)_4]^{2+}$ cation and a terephthalate anion. The geometry around the Ni^{II} ion is best described as distorted octahedral, and it associates with four water O atoms and the two N atoms of a 2,2′-bipyridine ligand (Fig. 1). It should be pointed out that ta^{2-} is a free anion and does not coordinate to the Ni atom, although IR data indicates that the ta^{2-} anion has a bridging coordination mode (Rogan *et al.*, 2000).



(I)

The cations and anions of (I) form a two-dimensional hydrogen-bonding network (Fig. 2). Each cation, simplified as $[Ni(H_2O)_4]^{2+}$, is linked to six terephthalate anions through hydrogen bonds (Fig. 3*a*), in which four of the six terephthalate anions are from one sheet of the two-dimensional network and the remaining two are from another sheet. Each terephthalate anion is in turn linked to six $[Ni(H_2O)_4]^{2+}$ cations through hydrogen bonds (Fig. 3*b*), four of which are from one sheet of the two-dimensional network and the remaining two are from another sheet. Each terephthalate carboxylate group is linked to three $[Ni(H_2O)_4]^{2+}$ cations. There are two hydrogen bonds between terephthalate atom O2 and two $[Ni(H_2O)_4]^{2+}$ cations from the same sheet. The second carboxylate O atom, O1, forms hydrogen bonds with two $[Ni(H_2O)_4]^{2+}$ cations from different sheets. Therefore, each terephthalate anion forms eight hydrogen bonds with $[Ni(H_2O)_4]^{2+}$ cations, producing a two-dimensional hydrogen-bonding network with double sheets.

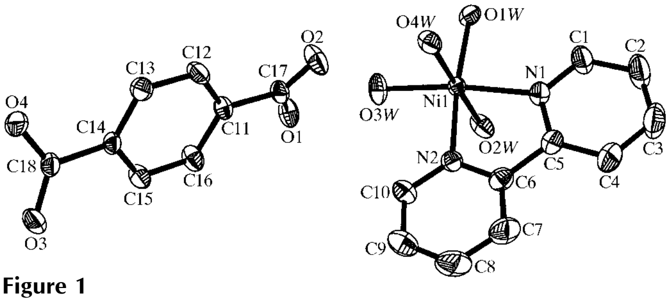


Figure 1
View of the title compound, showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

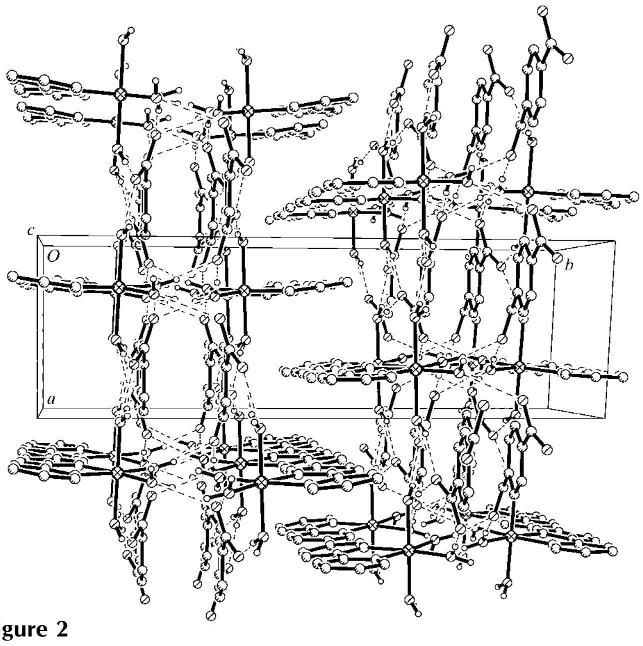


Figure 2
View of the two-dimensional hydrogen-bonding network in (I).

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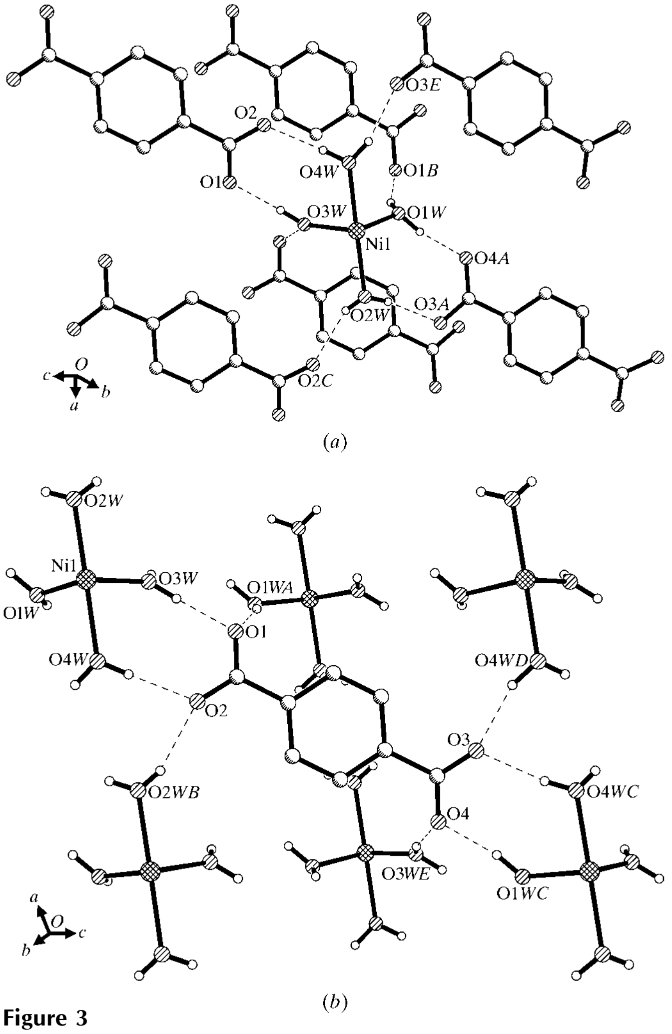

Figure 3
The hydrogen bonds formed (*a*) by the cations [symmetry codes: (*A*) $1 + x, y, -1 + z$; (*B*) $x, \frac{3}{2} - y, -\frac{1}{2} + z$; (*C*) $1 + x, y, z$; (*D*) $1 + x, \frac{3}{2} - y, -\frac{1}{2} + z$; (*E*) $x, y, -1 + z$] and (*b*) by the anions [symmetry codes: (*A*) $x, \frac{3}{2} - y, \frac{1}{2} + z$; (*B*) $-1 + x, y, z$; (*C*) $-1 + x, y, 1 + z$; (*D*) $x, y, 1 + z$; (*E*) $1 + x, \frac{3}{2} - y, \frac{1}{2} + z$]. The 2,2-bipyridine ligand has been omitted for clarity.

Experimental

A solution (10 ml) of dimethylformamide containing $Ni(NO_3)_2 \cdot 6H_2O$ (0.5 mmol) and H_2ta (0.5 mmol, 0.083 g) was added slowly to a solution (10 ml) of dimethylformamide containing 2,2′-bipyridine (0.5 mmol). The starting mixture was stirred for a few minutes and left to stand at room temperature for about one month. Green block-shaped crystals of (I) were obtained.

Table 1
Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1W-H1WA\cdots O1^{i}$	0.842 (18)	1.92 (2)	2.719 (3)	157 (3)
$O1W-H1WB\cdots O4^{ii}$	0.863 (18)	1.78 (2)	2.634 (3)	167 (4)
$O2W-H2WA\cdots O3^{ii}$	0.870 (18)	1.87 (2)	2.726 (3)	168 (4)
$O2W-H2WB\cdots O2^{iii}$	0.800 (18)	2.00 (2)	2.748 (3)	156 (4)
$O3W-H3WA\cdots O1$	0.893 (18)	1.753 (18)	2.644 (3)	175 (3)
$O3W-H3WB\cdots O4^{iv}$	0.837 (18)	1.91 (2)	2.722 (3)	163 (4)
$O4W-H4WA\cdots O3^{v}$	0.853 (18)	1.98 (2)	2.795 (3)	158 (4)
$O4W-H4WB\cdots O2$	0.853 (18)	1.899 (19)	2.745 (3)	171 (3)

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

Crystal data

$[Ni(C_{10}H_8N_2)(H_2O)_4](C_8H_4O_4)$
$M_r = 451.07$
Monoclinic, $P2_1/c$
$a = 7.5503$ (2) Å
$b = 23.5347$ (9) Å
$c = 11.1050$ (4) Å
$\beta = 102.427$ (2)°
$V = 1927.06$ (11) Å^3
$Z = 4$
$D_x = 1.555$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from all data
$\theta = 2.07$–29.97°
$\mu = 1.06$ mm^{-1}
$T = 293$ (2) K
Block, green
0.40 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.611$, $T_{max} = 0.810$
15 571 measured reflections
5600 independent reflections
3567 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 30.0°$
$h = -10 \rightarrow 10$
$k = -33 \rightarrow 13$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.126$
$S = 0.95$
5600 reflections
294 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.068P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.62$ e Å^{-3}
$\Delta\rho_{min} = -0.72$ e Å^{-3}

H atoms bonded to C atoms were treated as riding atoms, with a C—H distance of 0.93 Å. The H atoms of the water molecules were refined isotropically; see Table 1 for O—H distances.

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

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GD1242). Services for accessing these data are described at the back of the journal.

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