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μ-Benzene-1,2,4,5-tetracarboxylato-bis[triaqua(2,2′-bipyridine)nickel(II)] dihydrate

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In the title compound, $[Ni_2(C_{10}H_2O_8)(C_{10}H_8N_2)_2(H_2O)_6]\cdot 2H_2O$, the benzenetetracarboxylate anion, which lies on a center of symmetry, is monodentate to two bipyridine-chelated water-coordinated Ni atoms. The geometry of the Ni atom is that of an octahedron. The coordinated and uncoordinated water molecules are linked by hydrogen bonds into a network structure.

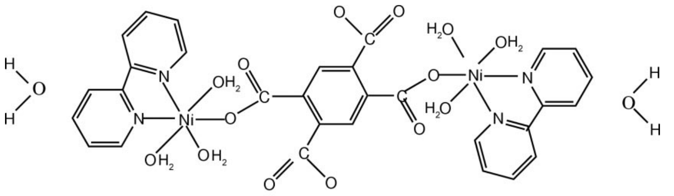
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.029
wR factor = 0.078
Data-to-parameter ratio = 11.7

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

Comment

The benzene-1,2,4,5-tetracarboxylate anion binds to metal atoms in a variety of bonding modes (Cao *et al.*, 2002), and a large number of coordination polymers have been structurally characterized (Hu *et al.*, 2003; Xiao & Zhu, 2003). These studies have been extended to the present binuclear nickel(II) complex, (I), in which the anion is present in a μ_2-bridging mode (Fig. 1). The anion lies on a special position of $\overline{1}$ site symmetry and binds to each Ni atom through only one carboxylate O atom. The geometry around the Ni atoms is that of an octahedron, being chelated by the heterocycle and also bonded to three water molecules. The coordinated and uncoordinated water molecules interact through hydrogen bonds (Table 2), generating a three-dimensional network.



(I)

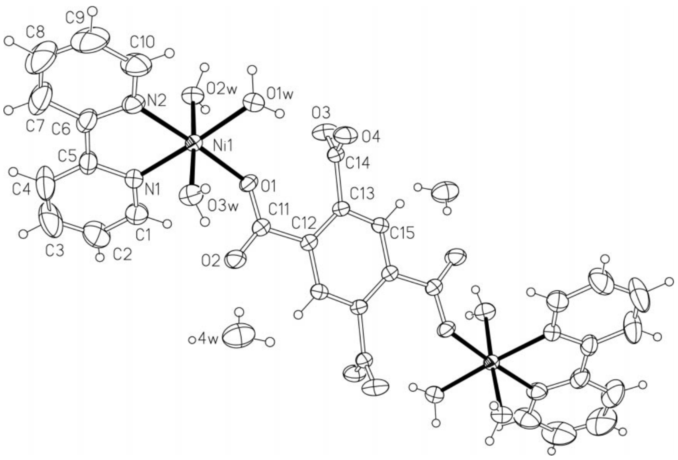


Figure 1
View of the structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

Experimental

A DMF (10 ml) solution of $Ni(NO_3)_2 \cdot 6H_2O$ (0.15 g, 0.5 mmol) and benzene-1,2,4,5-tetracarboxylic acid (0.13 g, 0.5 mmol) was mixed with a DMF solution (10 ml) of 2,2′-bipyridine (0.08 g, 0.5 mmol). After one month, green crystals separated from the solution.

Crystal data

$[Ni_2(C_{10}H_2O_8)(C_{10}H_8N_2)_2(H_2O)_6] \cdot 2H_2O$
$M_r = 824.03$
Triclinic, $P\overline{1}$
$a = 7.5839$ (4) Å
$b = 9.7257$ (6) Å
$c = 11.9698$ (7) Å
$\alpha = 76.927$ (1)°
$\beta = 87.388$ (1)°
$\gamma = 79.807$ (1)°
$V = 846.41$ (8) $Å^3$
$Z = 1$
$D_x = 1.617$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4405 reflections
$\theta = 2.5$–25.2°
$\mu = 1.19$ mm^{-1}
$T = 298$ (2) K
Prism, green
0.35 × 0.32 × 0.17 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.680$, $T_{max} = 0.823$
6271 measured reflections
3036 independent reflections
2903 reflections with $I > 2\sigma(I)$
$R_{int} = 0.013$
$\theta_{max} = 25.2°$
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.078$
$S = 1.02$
3036 reflections
259 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.4734P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e $Å^{-3}$
$\Delta\rho_{min} = -0.31$ e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °).

Ni1—N1	2.061 (2)	Ni1—O1*w*	2.075 (2)
Ni1—N2	2.065 (2)	Ni1—O2*w*	2.062 (2)
Ni1—O1	2.052 (1)	Ni1—O3*w*	2.082 (2)
N1—Ni1—N2	79.65 (7)	N2—Ni1—O3*w*	86.85 (7)
N1—Ni1—O1	97.78 (6)	O1—Ni1—O1*w*	85.00 (6)
N1—Ni1—O1*w*	176.98 (6)	O1—Ni1—O2*w*	89.71 (6)
N1—Ni1—O2*w*	88.26 (6)	O1—Ni1—O3*w*	91.54 (6)
N1—Ni1—O3*w*	89.09 (6)	O1*w*—Ni1—O2*w*	90.60 (6)
N2—Ni1—O1	176.99 (6)	O1*w*—Ni1—O3*w*	92.01 (6)
N2—Ni1—O1*w*	97.59 (7)	O2*w*—Ni1—O3*w*	177.20 (6)
N2—Ni1—O2*w*	91.80 (7)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O4	0.84 (1)	2.15 (1)	2.989 (2)	176 (2)
O1*w*—H1*w*2···O3^{i}	0.85 (1)	1.87 (1)	2.714 (2)	174 (2)
O2*w*—H2*w*2···O4^{i}	0.85 (1)	1.90 (1)	2.737 (2)	172 (2)
O2*w*—H2*w*1···O4*w*^{ii}	0.83 (2)	1.85 (2)	2.674 (2)	178 (2)
O3*w*—H3*w*1···O2	0.85 (1)	1.90 (1)	2.701 (2)	156 (2)
O3*w*—H3*w*2···O4^{iii}	0.84 (1)	1.93 (1)	2.746 (2)	163 (2)
O4*w*—H4*w*1···O2	0.85 (1)	1.83 (1)	2.676 (2)	173 (3)
O4*w*—H4*w*2···O3^{iv}	0.85 (1)	1.96 (1)	2.781 (3)	161 (3)

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

The aromatic H atoms were positioned geometrically and were included in the refinement in the riding model approximation (C—H = 0.93 Å). The water H atoms were located and refined with distance restraints [O—H = 0.85 (1) Å and H···H = 1.39 (1) Å]. The displacement parameters for all H atoms were $1.2U_{eq}$(C,O).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL*97.

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