

## Polymeric tetraqua(1,2,4,5-benzenetetracarboxylato)(pyrazine)nickel(II) dihydrate

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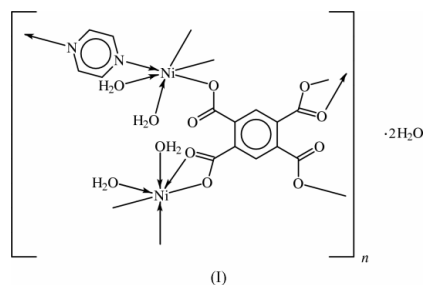
## Key indicators

Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$   
 $R$  factor = 0.065  
 $wR$  factor = 0.142  
Data-to-parameter ratio = 13.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The Ni atom in the title compound,  $\{[\text{Ni}_2(\text{C}_{10}\text{H}_2\text{O}_8)(\text{C}_4\text{H}_4\text{N}_2)(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}\}_n$ , exists in an octahedral  $\text{NO}_5\text{Ni}$  coordination environment that is defined by the two O atoms of a chelating carboxyl group, the O atom of a monodentate carboxyl group belonging to another carboxylato tetraanion, two water molecules and the N atom of the *N*-heterocycle. The tetracarboxylato anion and the pyrazine molecule are each located on a center of inversion. The bonding pattern leads to the formation of a layer structure; the layers are linked into a three-dimensional network by extensive hydrogen bonds involving the water molecules and the O atoms of the anionic unit.

## Comment

A number of adducts of nickel benzenepolycarboxylates with *N*-heterocycles have been reported (Li *et al.*, 2003; Yuan *et al.*, 2001). To this number has been added the 4,4'-bipyridine adduct of nickel terephthalate (Yang *et al.*, 2003a) and of nickel phthalate (Yang *et al.*, 2003b). The present pyrazine adduct, (I), of dinickel 1,2,4,5-benzenetetracarboxylate exists as the dihydrate (Fig. 1).



The Ni atom in (I) exists in an octahedral  $\text{NO}_5\text{Ni}$  environment that is defined by the two O atoms of a chelating  $-\text{CO}_2$  group, the O atom of a monodentate  $\text{CO}_2$  group of another tetraanion, two water molecules and the N atom of pyrazine (Table 1). The tetracarboxylato anion and the pyrazine molecule are each located on a center of inversion. The bonding pattern leads to the formation of layers; the layers are linked into a three-dimensional network by hydrogen bonds involving the water molecules and the O atoms of the anionic unit (Table 2).

## Experimental

1,2,4,5-Benzenetetracarboxylic acid anhydride (pyromellitic anhydride, 0.22 g, 1 mmol) was dissolved in water (15 ml) containing sodium hydroxide (0.16 g, 4 mmol). Nickel dinitrate hexahydrate

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(0.58 g, 2 mmol) and pyrazine (0.16 g, 2 mmol) dissolved in water (3 ml) were then added. The mixture was placed in a 20 ml Teflon-lined stainless-steel bomb. The bomb was heated at 453 K for 100 h. Crystals separated from the solution when the bomb was cooled down at a rate of 5 K h<sup>-1</sup>.

#### Crystal data

[Ni<sub>2</sub>(C<sub>10</sub>H<sub>2</sub>O<sub>8</sub>)(C<sub>4</sub>H<sub>4</sub>N<sub>2</sub>)-  
(H<sub>2</sub>O)<sub>4</sub>]-2H<sub>2</sub>O

*M<sub>r</sub>* = 555.72

Triclinic, *P*1

*a* = 7.2005 (5) Å

*b* = 8.0322 (5) Å

*c* = 9.3735 (6) Å

α = 96.175 (1)°

β = 101.872 (1)°

γ = 116.245 (1)°

*V* = 463.50 (5) Å<sup>3</sup>

*Z* = 1

*D<sub>x</sub>* = 1.991 Mg m<sup>-3</sup>

Mo *K*α radiation

Cell parameters from 2804

reflections

θ = 2.3–28.3°

μ = 2.12 mm<sup>-1</sup>

*T* = 298 (2) K

Irregular block, green

0.14 × 0.13 × 0.04 mm

#### Data collection

Bruker SMART APEX area-  
detector diffractometer

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

*T<sub>min</sub>* = 0.616, *T<sub>max</sub>* = 0.919

5415 measured reflections

2152 independent reflections

2055 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.041

θ<sub>max</sub> = 28.3°

*h* = -9 → 9

*k* = -10 → 10

*l* = -12 → 12

#### Refinement

Refinement on *F*<sup>2</sup>

*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.065

*wR* (*F*<sup>2</sup>) = 0.142

*S* = 1.25

2152 reflections

163 parameters

H atoms treated by a mixture of  
independent and constrained  
refinement

$w = 1/[\sigma^2(F_o^2) + (0.0629P)^2 + 0.259P]$

where  $P = (F_o^2 + 2F_c^2)/3$

(Δ/σ)<sub>max</sub> = 0.001

Δρ<sub>max</sub> = 0.95 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -0.65 e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Ni1—O1	2.126 (3)	Ni1—O1w	2.049 (3)
Ni1—O2	2.123 (3)	Ni1—O2w	2.025 (4)
Ni1—O3 <sup>i</sup>	2.014 (3)	Ni1—N1	2.068 (4)
O1—Ni1—O2	61.7 (1)	O2—Ni1—N1	85.8 (1)
O1—Ni1—O3 <sup>i</sup>	84.9 (1)	O3 <sup>i</sup> —Ni1—O1w	93.2 (1)
O1—Ni1—O1w	103.2 (1)	O3 <sup>i</sup> —Ni1—O2w	89.8 (1)
O1—Ni1—O2w	162.8 (1)	O3 <sup>i</sup> —Ni1—N1	173.6 (1)
O1—Ni1—N1	91.5 (1)	O1w—Ni1—O2w	93.4 (1)
O2—Ni1—O3 <sup>i</sup>	87.8 (1)	O1w—Ni1—N1	92.8 (1)
O2—Ni1—O1w	164.8 (1)	O2w—Ni1—N1	92.2 (2)
O2—Ni1—O2w	101.8 (1)		

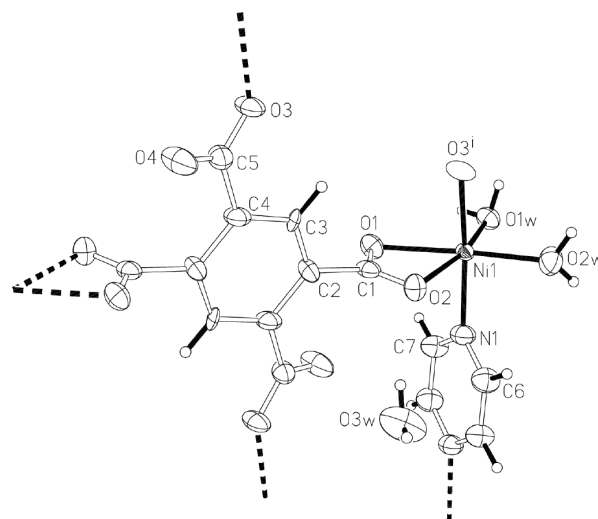
Symmetry code: (i) 1 - *x*, 1 - *y*, 2 - *z*.

**Table 2**

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1w—H1w2...O1 <sup>ii</sup>	0.85 (1)	1.87 (3)	2.660 (5)	155 (5)
O1w—H1w1...O4 <sup>i</sup>	0.84 (1)	1.82 (2)	2.621 (5)	157 (5)
O2w—H2w2...O1w <sup>iii</sup>	0.85 (1)	1.96 (1)	2.807 (5)	176 (6)
O2w—H2w1...O3w <sup>iv</sup>	0.85 (1)	1.90 (1)	2.744 (5)	176 (6)
O3w—H3w1...O2	0.85 (1)	2.26 (3)	3.047 (5)	155 (6)
O3w—H3w2...O3 <sup>v</sup>	0.85 (1)	2.02 (1)	2.866 (5)	174 (7)

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



**Figure 1**

ORTEPII (Johnson, 1976) plot of a segment of the title structure, with displacement ellipsoids at the 75% probability level. [Symmetry code: (i) 1 - *x*, 1 - *y*, 2 - *z*.]

The use of too small a value for the  $\theta$ -dependent absorption correction in *SADABS* (Sheldrick, 1996) led to non-positive definite displacement parameters for several atoms, and a compromise value of 0.5 was used, for which parameters of only one atom (C3) were non-positive definite. The displacement parameter of this atom was restrained to be close to isotropic. The aromatic H atoms were positioned geometrically (C—H = 0.93 Å) and were included in the refinement in the riding-model approximation, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The water H atoms were located and refined with restraints of O—H = 0.85 (1) Å, H...H = 1.39 (1) Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ .

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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