Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Poly[diaquadi-μ_3-malonato-μ-pyrazine-dinickel(II)]

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Received 21 July 2005
Accepted 18 August 2005
Online 27 August 2005

Key indicators

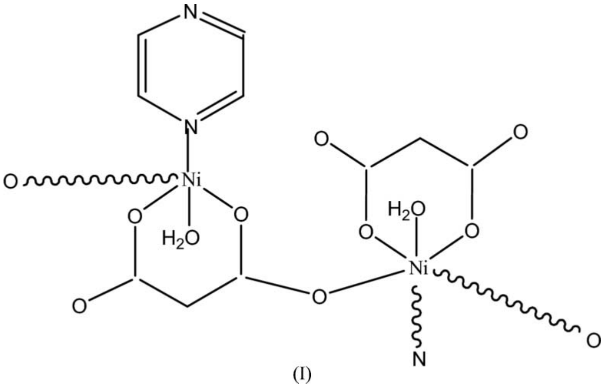
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.033
wR factor = 0.089
Data-to-parameter ratio = 10.9

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

The title compound, $[Ni_2(C_3H_2O_4)_2(C_4H_4N_2)(H_2O)_2]_n$, has been prepared from the hydrothermal reaction of nickel(II) chloride, malonic acid and pyrazine. The Ni^{II} atoms are linked *via* coordinated malonates, forming a two-dimensional network with cavities of 6.14 × 5.60 Å. These sheet structures are further connected into a three-dimensional network by bridging pyrazine ligands which have inversion symmetry, the mean distance between the layers being 7.39 Å. The coordination geometry around the Ni^{II} atom is a tetragonally elongated octahedron, with pyrazine N and aqua O atoms at the apical positions.

Comment

In recent years, dicarboxylic acids have been widely used as polydentate ligands, which undergo various metal chelation reactions to form transition or rare earth metal complexes with interesting properties in materials science (Church & Halvorson, 1959; Chung *et al.*, 1971) and in biological systems (Okabe & Oya, 2000; Serre *et al.*, 2005; Pocker & Fong, 1980; Scapin *et al.*, 1997). For example, Kim *et al.* (2001) focused on the syntheses of transition metal complexes containing benzene dicarboxylate and rigid aromatic pyridine ligands in order to study their electronic conductivity and magnetic properties. The importance of transition metal dicarboxylate complexes in materials science and biological systems prompted us to pursue synthetic strategies for these compounds, using malonate as a polydentate ligand and pyrazine as a rigid aromatic ligand. In this paper, we report the synthesis and X-ray crystal structure analysis of the title compound, $[Ni_2(malonate)_2(pyrazine)(H_2O)_2]_n$, (I).



(I)

The Ni^{II} atom of (I) has sixfold coordination, chelated by two O atoms from one malonate ligand to form a six-membered boat-type ring, and by two O atoms from two neighbouring malonates, one aqua molecule and one N atom

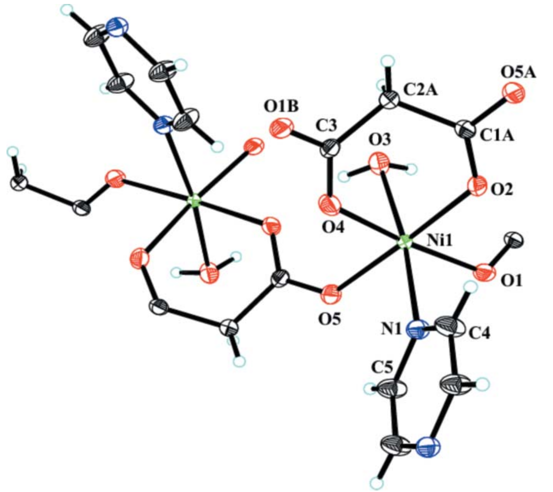


Figure 1
A view of the structure of (I), showing 50% probability displacement ellipsoids. Atoms labelled with the suffix A or B are at the symmetry positions ($\frac{1}{2}+x$, $\frac{3}{2}-y$, $z-\frac{1}{2}$) and ($\frac{1}{2}+x$, $\frac{3}{2}-y$, $z+\frac{1}{2}$), respectively. Unlabelled atoms are at the symmetry position **? [Please provide symmetry code]**

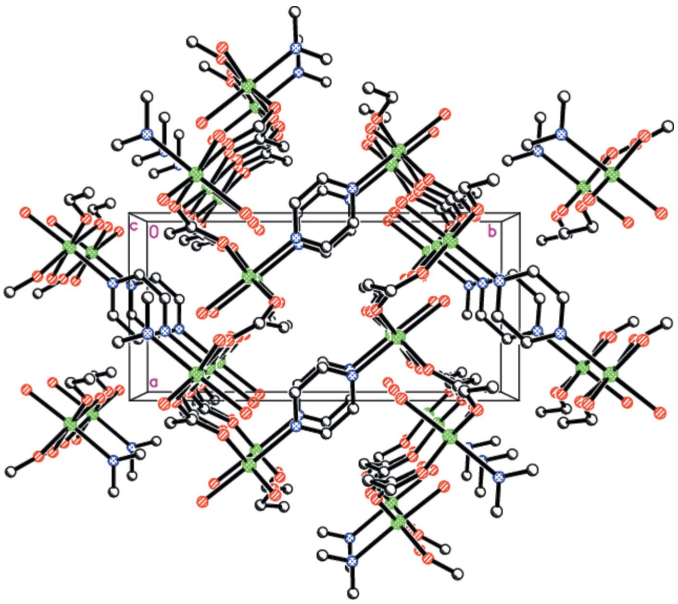


Figure 2
A packing diagram for (I), viewed along the *c* axis. H atoms have been omitted.

from the bridging pyrazine ligand (Fig. 1). The coordinating atoms around the Ni^{II} atom exhibit a tetragonally elongated octahedral geometry, the equatorial plane of which is composed of atoms O1/O2/O4/O5, with the deviations for these four atoms and for Ni1 being less than 0.05 Å. The apical positions are occupied by aqua O3 and pyrazine N1 atoms. The Ni—O(carboxylate) bond lengths are in the range 2.050 (2)–2.079 (2) Å (Table 1), whereas the Ni—O3 and Ni—N distances in the axial direction are much longer [2.205 (3) and 2.266 (3) Å, respectively].

The packing diagram for (I) is shown in Fig. 2. If the pyrazine bridges are neglected, a two-dimensional network is formed by the [Ni(malonate)(H_2O)] moieties parallel to the (010) plane. There are hydrogen bonds (Table 2) between the aqua and malonate ligands in this network. The bridging mode of the malonate is similar to those observed in other nickel compounds (Gil de Muro *et al.*, 1999; Xiao *et al.*, 2004; Deigado *et al.*, 2004; Ruiz-Perez *et al.*, 2000; Zheng & Xie, 2004).

Experimental

A mixture of nickel(II) chloride (0.5 mmol), malonic acid (0.5 mmol), sodium hydroxide (1 mmol), pyrazine (1 mmol) and H_2O (8 ml) in a 25 ml Teflon-lined stainless steel autoclave was heated at 443 K for 2 d and then cooled to room temperature. Green columnar crystals of (I) were obtained with a yield of 35%. Analysis, calculated for $C_{10}H_{12}N_2Ni_2O_{10}$: C 27.42, N 6.40, Ni 13.41%; found: C 27.45, N 6.38, Ni 13.38%.

Crystal data

$[Ni_2(C_3H_2O_4)_2(C_4H_4N_2)(H_2O)_2]$
$M_r = 437.6$
Monoclinic, $P2_1/n$
$a = 6.9783$ (5) Å
$b = 14.5612$ (9) Å
$c = 7.3348$ (5) Å
$\beta = 92.181$ (2)°
$V = 744.77$ (9) Å^3
$Z = 2$
$D_x = 1.951$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1338 reflections
$\theta = 1.7$–25.2°
$\mu = 2.59$ mm^{-1}
$T = 293$ (2) K
Column, green
0.42 × 0.37 × 0.33 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.375$, $T_{max} = 0.426$
2429 measured reflections
1338 independent reflections
1118 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 25.2°$
$h = -8 \rightarrow 3$
$k = -13 \rightarrow 17$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.089$
$S = 1.00$
1338 reflections
123 parameters
Only H-atom U_{iso} values refined
$w = 1/[\sigma^2(F_o^2) + (0.0643P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997a)
Extinction coefficient: 0.018 (3)

Table 1
Selected geometric parameters (Å, °).

Ni1—O5	2.050 (2)	Ni1—O4	2.079 (2)
Ni1—O1	2.066 (2)	Ni1—O3	2.205 (3)
Ni1—O2	2.076 (2)	Ni1—N1	2.266 (3)
O5—Ni1—O1	97.24 (10)	O2—Ni1—O3	91.43 (10)
O5—Ni1—O2	173.93 (9)	O4—Ni1—O3	86.81 (11)
O1—Ni1—O2	88.19 (10)	O5—Ni1—N1	84.79 (9)
O5—Ni1—O4	90.12 (10)	O1—Ni1—N1	90.39 (9)
O1—Ni1—O4	172.21 (9)	O2—Ni1—N1	92.46 (10)
O2—Ni1—O4	84.35 (9)	O4—Ni1—N1	87.72 (10)
O5—Ni1—O3	90.76 (9)	O3—Ni1—N1	172.94 (10)
O1—Ni1—O3	95.62 (10)		

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O3—H5⋯O2^{i}	0.86 (2)	1.91 (4)	2.693 (3)	151 (4)
O3—H6⋯O4^{ii}	0.85 (2)	1.82 (5)	2.623 (3)	155 (7)

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

H atoms were located in difference density maps and refined isotropically with restrained bond distances [O3—H5/H6 = 0.85 (2) Å, H5⋯H6 = 1.38 (2) Å and Ni1⋯H6 = 2.5 (5) Å for the water molecule; C—H = 0.85 (2) Å].

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* **[or SAINT?]**; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors thank Liaocheng University for financial support and Professor Jianmin Dou for his help.

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