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Diaquabis(5-methylpyrazine-2-carboxylato-κ^2N^1,O)-nickel(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.035
wR factor = 0.091
Data-to-parameter ratio = 14.2

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

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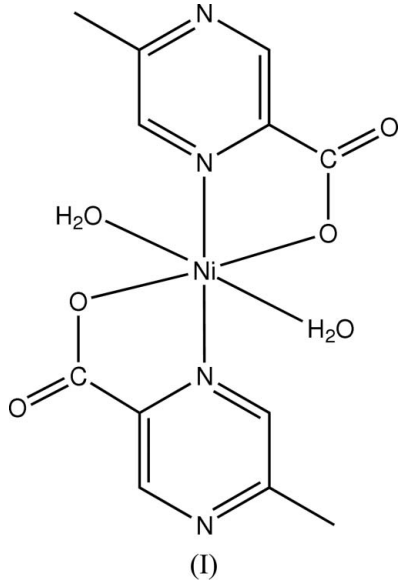
In the title compound, $[Ni(C_6H_5N_2O_2)_2(H_2O)_2]$, the Ni atom is located on a centre of inversion and shows a distorted octahedral coordination geometry. Two aqua ligands occupy the axial positions and two O atoms and two N atoms of the two chelating 5-methylpyrazine-2-carboxylate ligands are located in the equatorial plane. Intermolecular hydrogen bonds between water molecules and organic ligands link molecules into a two-dimensional network.

Comment

In the past decade, much attention has been paid to the design and synthesis of self-assembling systems with organic ligands containing *N*- and *O*-donors (Steiner, 2002; Zafar *et al.*, 2000; Seto *et al.*, 1990). 5-Methylpyrazine-2-carboxylate ($Mepyzca^-$) is one such ligand and several crystal structures of complexes containing the Mepyzca ligand have been reported (Ciurtin *et al.*, 2001, 2003; Dong *et al.*, 2000; Chapman *et al.*, 2002; Ptasiewicz-Bak *et al.*, 2000). We report here the synthesis and crystal structure of the title complex, (I) (Fig. 1).



(I)

In (I), the Ni atom is located on a crystallographic inversion centre and adopts a distorted octahedral coordination geometry. The coordination environment is defined by two pyrazine nitrogen donors and two oxygen donors from the carboxylate groups located in the equatorial plane and two aqua O-atom donors located in the axial positions (Fig. 1). Selected bond lengths and angles are shown in Table 1. Intermolecular O—H···O hydrogen bonds between water

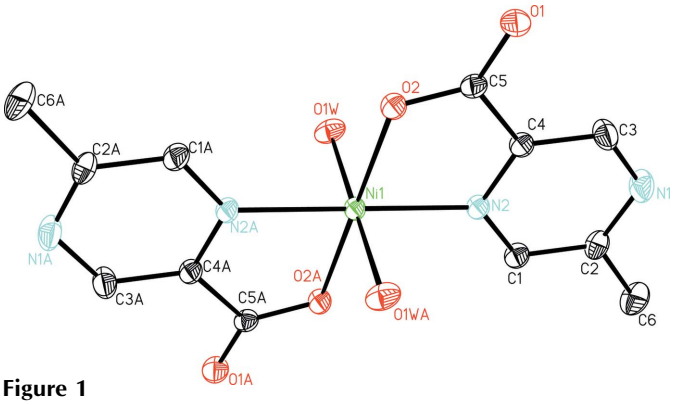


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level. H atoms are shown as spheres of arbitrary radii. H atoms have been omitted. [Symmetry code: (A) $-x+1, -y, -z+1$.]

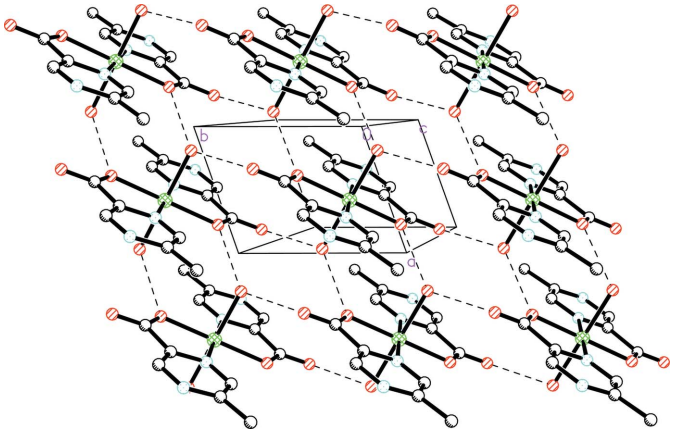


Figure 2
The crystal packing. Dashed lines indicate hydrogen bonds. H atoms have been omitted for clarity.

molecules and carboxylate groups connect the molecules of (I) into a two-dimensional network (Table 2 and Fig. 2).

Experimental

All chemicals were obtained from commercial sources and used without further purification. To a solution of $NiCl_2\cdot 6H_2O$ (23.7 mg, 0.1 mmol) in 10 ml of water, a solution of 5-methylpyrazine-2-carboxylic acid (13.8 mg, 0.1 mmol) in 5 ml of EtOH was added. The resulting solution was stirred at room temperature for 30 min and then filtered. Blue crystals were obtained by slow evaporation of the resulting solution after two weeks.

Crystal data

$[Ni(C_6H_5N_2O_2)_2(H_2O)_2]$
$M_r = 368.96$
Triclinic, $P\overline{1}$
$a = 5.1464\ (10)$ Å
$b = 6.4218\ (13)$ Å
$c = 12.142\ (2)$ Å
$\alpha = 104.38\ (3)^\circ$
$\beta = 90.60\ (3)^\circ$
$\gamma = 109.44\ (3)^\circ$
$V = 364.64\ (15)$ Å^3
$Z = 1$
$D_x = 1.680$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.37$ mm^{-1}
$T = 298\ (2)$ K
Block, blue
0.19 × 0.16 × 0.14 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: integration (*SADABS*; Bruker, 2000)
$T_{min} = 0.770$, $T_{max} = 0.824$
2363 measured reflections
1617 independent reflections
1525 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 28.2^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.091$
$S = 1.06$
1617 reflections
114 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2 + 0.2144P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.015$
$\Delta\rho_{max} = 0.46$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.042 (2)

Table 1
Selected geometric parameters (Å, °).

Ni1—N2	2.058 (2)	Ni1—O1*W*	2.068 (2)
Ni1—O2	2.0584 (17)		
N2—Ni1—O2	80.44 (7)	N2^{i}—Ni1—O1*W*	87.93 (9)
N2^{i}—Ni1—O2	99.56 (7)	O2—Ni1—O1*W*	90.56 (8)
N2—Ni1—O1*W*	92.07 (9)	O2^{i}—Ni1—O1*W*	89.44 (8)

Symmetry code: (i) $-x+1, -y, -z+1$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WB*···O1^{ii}	0.77 (2)	1.95 (4)	2.683 (3)	165 (3)
O1*W*—H1*WA*···O2^{iii}	0.77 (2)	1.98 (4)	2.741 (3)	158 (4)

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

H atoms bound to C atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å for aromatic and 0.96 Å for methyl H atoms, and with $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms. The water H atoms were located in a difference Fourier map, and were refined with a distance restraint of O—H = 0.77 (2) Å; their displacement parameters were freely refined.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; 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: *SHELXL97*.

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