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Bis(pyrazine-2-carboxylato-κ^2N^1,O^2)-nickel(II) dihydrate

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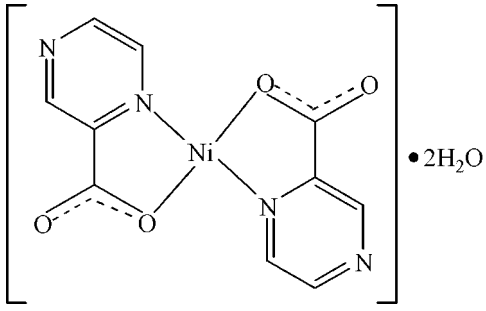
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.039; wR factor = 0.096; data-to-parameter ratio = 11.7.

In the title compound, $[Ni(C_5H_3N_2O_2)_2]\cdot 2H_2O$, the Ni^{II} cation is four-coordinated by two N and two O atoms belonging to two pyrazine-2-carboxylate ligands. The Ni^{II} atom occupies a special position at a centre of symmetry. Hydrogen bonds between water molecules, and between water molecules and carboxylate O atoms, stabilize the crystal structure.

Related literature

For related literature, see: Church & Halvorson (1959); Chung *et al.* (1971); Okabe & Oya (2000); Serre *et al.* (2005); Pocker & Fong (1980); Scapin *et al.* (1997).



Experimental

Crystal data

$[Ni(C_5H_3N_2O_2)_2]\cdot 2H_2O$
M_r = 340.93
Triclinic, $P\overline{1}$
a = 5.5576 (6) Å
b = 7.3252 (9) Å
c = 9.3021 (11) Å
α = 75.065 (2)°
β = 84.298 (2)°
γ = 71.503 (2)°
V = 346.93 (7) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.43 mm^{-1}
T = 293 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Bruker APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.870, T_{max} = 0.870
1705 measured reflections
1208 independent reflections
1111 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.096
S = 1.00
1208 reflections
103 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H2W···O1W^{i}	0.83 (5)	2.52 (6)	3.071 (9)	125 (6)
O1W—H1W···O2^{ii}	0.84 (2)	2.11 (3)	2.941 (4)	167 (7)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2122).

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supplementary materials

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Bis(pyrazine-2-carboxylato-κ^2N^1,O^2)nickel(II) dihydrate

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Comment

In recent years carboxylic acids have been widely used as polydentate ligands, which can coordinate to transition or rare earth ions yielding complexes with interesting properties that are useful 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). Herein, we report the synthesis and X-ray crystal structure analysis of the title compound bis(pyrazine-2-carboxylato)nickel(II) hydrate (Fig. 1). The nickel cation is tetra-coordinated by two O an d two N atoms belonging to two pyrazine-2-carboxylate. Hydrogen bonds between symmetry operated water molecules, and water molecule and carboxylate oxygen atom stablize the crystal structure (Table 1 and Fig. 2).

Experimental

The 8 ml etanol solution of nickel acetate (0.5 mmol), pyrazine-2-carboxylic acid (1.0 mmol) in a 25 ml Teflon-lined stainless steel autoclave was kept at 423 K for three days. Green crystals were obtained after cooling to room temperature with a yield of 35%. Anal. Calc. for $C_{10}H_{10}N_4Ni$: C 35.19, H 2.93, N 16.42%; Found: C 35.11, H 2.97, N 16.38%.

Refinement

The H atoms of the water molecule were located from difference density maps and were refined with distance restraints of d(H–H) = 1.38 (2)Å and d(O–H) = 0.82 (2) Å. All other H atoms were placed in calculated positions with a C—H bond distance of 0.93 Å and $U_{iso}(H) = 1.2U_{eq}$ of the respective carrier atom.

Figures

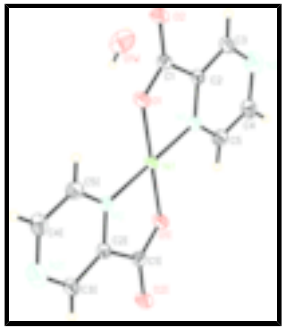

Fig. 1. The molecular structure of (I) with the 30% probability displacement ellipsoids. Symmetry operator i: 1 *x*, *y*, *z* + 1.

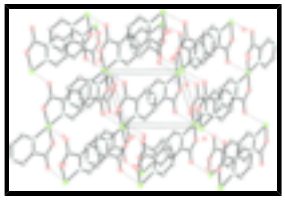

Fig. 2. The packing diagram of the title compound along the direction [010].

Bis(pyrazine-2-carboxylato-κ^2*N*^{1},*O*^{2})nickel(II) dihydrate

Crystal data

$[Ni(C_5H_3N_2O_2)_2]\cdot 2H_2O$	$Z = 1$
$M_r = 340.93$	$F_{000} = 174$
Triclinic, $P\bar{1}$	$D_x = 1.632$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.5576$ (6) Å	Cell parameters from 1208 reflections
$b = 7.3252$ (9) Å	$\theta = 2.3$–25.0º
$c = 9.3021$ (11) Å	$\mu = 1.43$ mm^{-1}
$\alpha = 75.065$ (2)º	$T = 293$ (2) K
$\beta = 84.298$ (2)º	Cube, green
$\gamma = 71.503$ (2)º	0.10 × 0.10 × 0.10 mm
$V = 346.93$ (7) Å^3	

Data collection

Bruker APEX II CCD area-detector diffractometer	1208 independent reflections
Radiation source: fine-focus sealed tube	1111 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.050$
$T = 293(2)$ K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 2.3$º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -6\rightarrow 5$
$T_{min} = 0.870$, $T_{max} = 0.870$	$k = -8\rightarrow 8$
1705 measured reflections	$l = -8\rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.096$	$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
1208 reflections	$\Delta\rho_{max} = 0.54$ e Å^{-3}

103 parameters	$\Delta\rho_{min} = -0.51$ e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	1.0000	0.0000	1.0000	0.0297 (2)
C1	0.4654 (6)	0.1781 (4)	1.0641 (4)	0.0332 (7)
C2	0.5285 (6)	0.3005 (4)	0.9152 (4)	0.0317 (7)
C3	0.3444 (6)	0.4682 (5)	0.8416 (4)	0.0385 (8)
H3	0.1797	0.5093	0.8789	0.046*
C4	0.6886 (8)	0.4949 (5)	0.6507 (4)	0.0481 (9)
H4	0.7394	0.5640	0.5604	0.058*
C5	0.8593 (7)	0.3250 (5)	0.7289 (4)	0.0412 (8)
H5	1.0228	0.2770	0.6919	0.049*
N1	0.7810 (5)	0.2302 (4)	0.8615 (3)	0.0326 (6)
N2	0.4262 (7)	0.5699 (5)	0.7071 (4)	0.0652 (10)
O1	0.6702 (4)	0.0410 (3)	1.1256 (2)	0.0378 (5)
O2	0.2286 (4)	0.2137 (3)	1.1166 (3)	0.0455 (6)
O1W	0.2352 (8)	0.0433 (7)	0.4397 (4)	0.1007 (13)
H1W	0.212 (13)	0.087 (10)	0.347 (3)	0.151*
H2W	0.369 (8)	−0.051 (8)	0.455 (7)	0.151*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0229 (3)	0.0247 (3)	0.0327 (3)	−0.0004 (2)	0.0048 (2)	−0.0021 (2)
C1	0.0315 (17)	0.0276 (15)	0.0401 (18)	−0.0068 (13)	0.0029 (13)	−0.0115 (13)
C2	0.0307 (16)	0.0260 (15)	0.0393 (18)	−0.0074 (13)	0.0009 (13)	−0.0114 (13)
C3	0.0374 (18)	0.0293 (16)	0.0450 (19)	−0.0040 (14)	−0.0017 (14)	−0.0100 (14)
C4	0.061 (2)	0.0363 (18)	0.041 (2)	−0.0155 (17)	−0.0010 (17)	0.0021 (15)
C5	0.0383 (18)	0.0409 (18)	0.0406 (19)	−0.0125 (15)	0.0048 (15)	−0.0046 (15)
N1	0.0315 (14)	0.0272 (13)	0.0365 (15)	−0.0072 (11)	0.0026 (11)	−0.0065 (11)
N2	0.074 (3)	0.0471 (19)	0.067 (2)	−0.0094 (17)	−0.0119 (19)	−0.0083 (17)

O1	0.0340 (12)	0.0307 (11)	0.0390 (13)	−0.0014 (9)	0.0043 (10)	−0.0043 (10)
O2	0.0343 (13)	0.0406 (13)	0.0530 (15)	−0.0033 (10)	0.0137 (11)	−0.0121 (11)
O1W	0.106 (3)	0.127 (4)	0.059 (2)	−0.051 (3)	−0.002 (2)	0.014 (2)

Geometric parameters (Å, °)

Ni1—N1	1.968 (3)	C3—N2	1.395 (5)
Ni1—N1^{i}	1.968 (3)	C3—H3	0.9300
Ni1—O1^{i}	2.054 (2)	C4—C5	1.378 (5)
Ni1—O1	2.054 (2)	C4—N2	1.481 (5)
C1—O1	1.319 (4)	C4—H4	0.9300
C1—O2	1.326 (4)	C5—N1	1.355 (4)
C1—C2	1.519 (4)	C5—H5	0.9300
C2—C3	1.390 (5)	O1W—H1W	0.84 (2)
C2—N1	1.421 (4)	O1W—H2W	0.83 (5)
N1—Ni1—N1^{i}	180.00 (14)	N2—C3—H3	122.6
N1—Ni1—O1^{i}	99.06 (9)	C5—C4—N2	121.5 (3)
N1^{i}—Ni1—O1^{i}	80.94 (9)	C5—C4—H4	119.3
N1—Ni1—O1	80.94 (9)	N2—C4—H4	119.3
N1^{i}—Ni1—O1	99.06 (9)	N1—C5—C4	117.8 (3)
O1^{i}—Ni1—O1	180.0	N1—C5—H5	121.1
O1—C1—O2	127.9 (3)	C4—C5—H5	121.1
O1—C1—C2	111.3 (2)	C5—N1—C2	120.9 (3)
O2—C1—C2	120.8 (3)	C5—N1—Ni1	124.8 (2)
C3—C2—N1	124.7 (3)	C2—N1—Ni1	114.3 (2)
C3—C2—C1	120.0 (3)	C3—N2—C4	120.5 (3)
N1—C2—C1	115.3 (3)	C1—O1—Ni1	117.65 (19)
C2—C3—N2	114.7 (3)	H1W—O1W—H2W	110 (3)
C2—C3—H3	122.6		

Symmetry codes: (i) −*x*+2, −*y*, −*z*+2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H2W···O1W^{ii}	0.83 (5)	2.52 (6)	3.071 (9)	125 (6)
O1W—H1W···O2^{iii}	0.84 (2)	2.11 (3)	2.941 (4)	167 (7)

Symmetry codes: (ii) −*x*+1, −*y*, −*z*+1; (iii) *x*, *y*, *z*−1.

Fig. 1

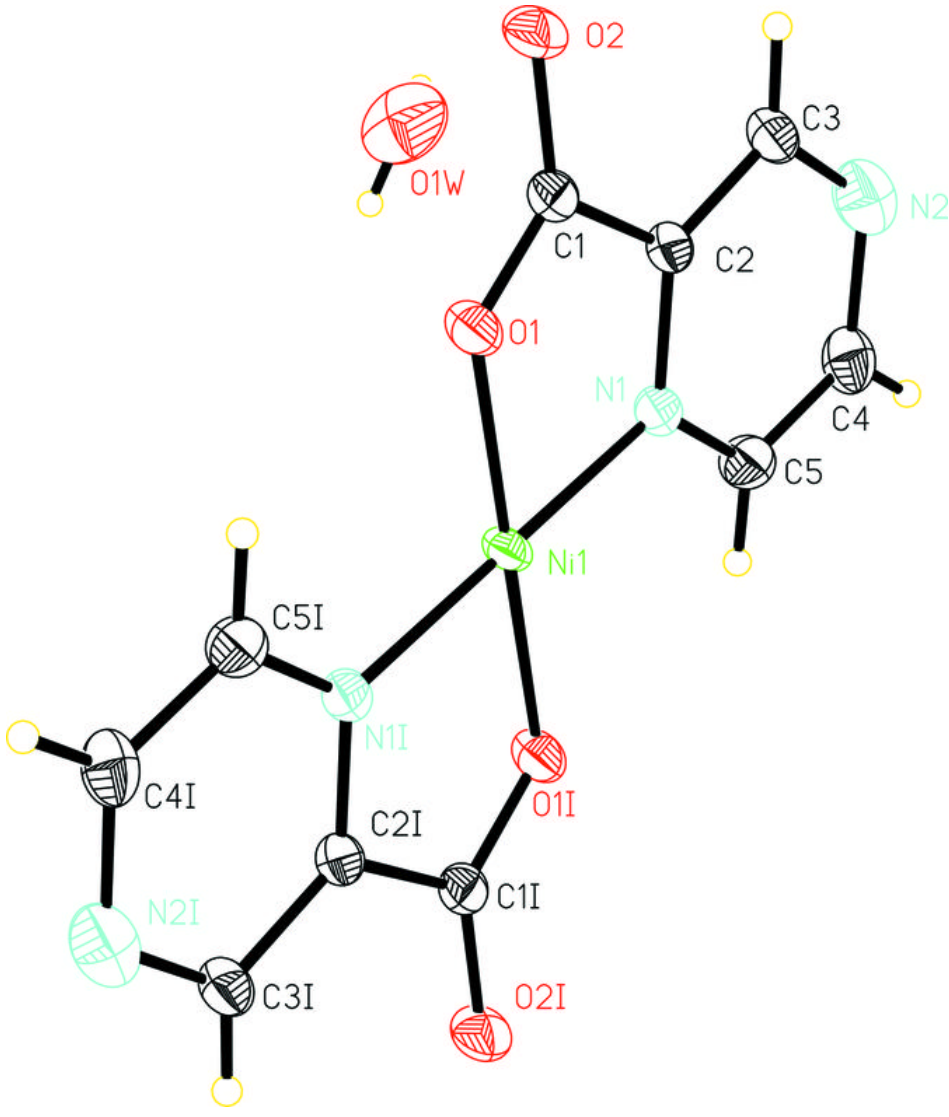
O2
O1W
C3
N2
C1
C2
O1
N1
C4
C5
Ni1
C5I
N1I
O1I
C4I
C2I
C1I
N2I
C3I
O2I

Fig. 2