

Tetraaquabis(2-oxo-1,2-dihydroquinoline-4-carboxylato- κO^4)nickel(II)

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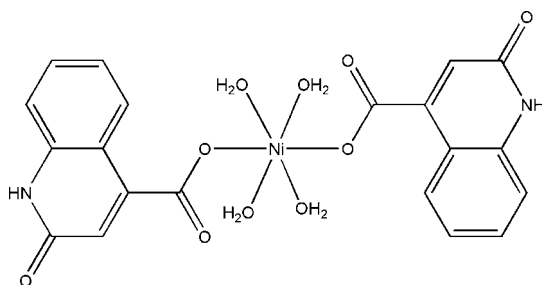
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(C-C) = 0.004$ Å; R factor = 0.034; wR factor = 0.121; data-to-parameter ratio = 14.9.

In the title compound, $[Ni(C_{10}H_6NO_3)_2(H_2O)_4]$, the central Ni^{II} atom is located on an inversion center and coordinated in a slightly distorted octahedral geometry by two O atoms from two 2-oxo-1,2-dihydroquinoline-4-carboxylate ligands and four water molecules, all of which act as monodentate ligands. The crystal structure features an extensive network of intermolecular hydrogen-bonding interactions ($O-H\cdots O$ and $N-H\cdots O$) and offset face-to-face $\pi-\pi$ stacking interactions [centroid-centroid distances = 3.525 (3) and 3.281 (5) Å].

Related literature

For related literature, see: Bai *et al.* (2007); Bu *et al.* (2005); Liu (2007); Pang *et al.* (2007); Wu *et al.* (2007); Xiong *et al.* (2000); Zhang *et al.* (2007).



Experimental

Crystal data

$[Ni(C_{10}H_6NO_3)_2(H_2O)_4]$
 $M_r = 507.07$
Triclinic, $P\bar{1}$
 $a = 7.105$ (5) Å
 $b = 8.507$ (5) Å
 $c = 9.216$ (5) Å
 $\alpha = 108.723$ (5)°
 $\beta = 108.396$ (5)°

$\gamma = 90.840$ (5)°
 $V = 496.4$ (5) Å³
 $Z = 1$
Mo $K\alpha$ radiation
 $\mu = 1.04$ mm⁻¹
 $T = 293$ (2) K
 $0.5 \times 0.4 \times 0.3$ mm

Data collection

Bruker SMART APEXII CCD
area-detector diffractometer
Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)
 $T_{min} = 0.601$, $T_{max} = 0.721$

3041 measured reflections
2250 independent reflections
2064 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.015$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.121$
 $S = 1.02$
2250 reflections

151 parameters
H-atom parameters constrained
 $\Delta\rho_{max} = 0.40$ e Å⁻³
 $\Delta\rho_{min} = -0.57$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ni1—O1	2.007 (2)	Ni1—O2W	2.117 (2)
Ni1—O1W	2.083 (2)		
O1—Ni1—O1W	89.31 (10)	O1W—Ni1—O2W	89.05 (9)
O1—Ni1—O1W ⁱⁱ	90.69 (10)	O1W ⁱⁱ —Ni1—O2W	90.95 (9)
O1—Ni1—O2W	88.35 (8)	O1—Ni1—O2W ⁱⁱ	91.65 (8)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A \cdots O2W ⁱⁱ	0.86	2.18	3.031 (3)	173
O1W—H1 \cdots O2 ⁱⁱⁱ	0.85	1.94	2.783 (3)	169
O1W—H2 \cdots O3 ^{iv}	0.85	1.89	2.722 (3)	164
O2W—H3 \cdots O2 ⁱ	0.85	1.90	2.709 (3)	158
O2W—H4 \cdots O3 ^v	0.85	1.98	2.767 (3)	154

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL-Plus (Siemens, 1990); software used to prepare material for publication: SHELXTL-Plus.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2104).

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supplementary materials

Acta Cryst. (2008). E64, m389-m390 [doi:10.1107/S1600536807065671]

Tetraaquabis(2-oxo-1,2-dihydroquinoline-4-carboxylato- κO^4)nickel(II)

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Comment

Recently, the complexes based on quinoline-4-carboxylic acid have been reported (Bu *et al.*, 2005; Xiong *et al.*, 2000). However, the compounds built from 2-oxo-1,2-dihydroquinoline-4-carboxylic acid (dhqc) and transition metals have not been reported. When 2-hydroxyquinoline-4-carboxylic acid (hqc) and NiCl₂ were employed as starting materials, the title compound, as shown in Fig. 1, was obtained. X-ray diffraction analysis has revealed that hqc exists mainly in the form of its tautomer dhqc, because the proton transfers from hydroxyl O atom to N atom under alkaline condition. Similar to the most mononuclear Ni complexes reported previously (Bai *et al.*, 2007; Liu, 2007; Pang *et al.*, 2007; Wu *et al.*, 2007; Zhang *et al.*, 2007), the Ni^{II} atom in the title compound, lying on an inversion center, is six-coordinated by four water molecules and two O atoms from two dhqc ligands (Table 1), forming a slightly distorted octahedral geometry. The molecules are linked into a three-dimensional network by a combination of intermolecular hydrogen bonds (O—H \cdots O and N—H \cdots O) (Table 2) and offset face-to-face π - π stacking interactions [centroid-to-centroid distances 3.525 (3) and 3.281 (5) Å].

Experimental

A mixture of 2-hydroxyquinoline-4-carboxylic acid (0.945 g, 5 mmol), NaOH(0.4 g, 10 mmol) and NiCl₂·6H₂O (2.3 g, 10 mmol) in water (50 ml) was boiled for 20 min with stirring. Then the mixture was cooled to room temperature. The resulting solution was filtered and allowed to stand. After a week, green crystals of the title compound were obtained.

Refinement

H atoms on C atoms and N atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å, N—H = 0.86 Å and $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{C},\text{N})$. Water H atoms were located in a difference Fourier map and refined with a restraint of O—H = 0.85 (1) Å, and $U_{\text{iso}}(\text{H})=1.5U_{\text{eq}}(\text{O})$.

Figures

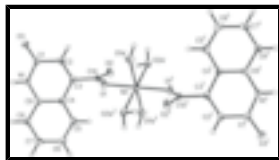


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) 1 - x, 2 - y, 1 - z.]

Tetraaquabis(2-oxo-1,2-dihydroquinoline-4-carboxylato- κO^4)nickel(II)

Crystal data

[Ni(C₁₀H₆NO₃)₂(H₂O)₄]

Z = 1

supplementary materials

$M_r = 507.07$	$F_{000} = 262$
Triclinic, $P\bar{1}$	$D_x = 1.696 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 7.105 (5) \text{ \AA}$	$\lambda = 0.71069 \text{ \AA}$
$b = 8.507 (5) \text{ \AA}$	Cell parameters from 2250 reflections
$c = 9.216 (5) \text{ \AA}$	$\theta = 1.3\text{--}26.0^\circ$
$\alpha = 108.723 (5)^\circ$	$\mu = 1.04 \text{ mm}^{-1}$
$\beta = 108.396 (5)^\circ$	$T = 293 (2) \text{ K}$
$\gamma = 90.840 (5)^\circ$	Block, green
$V = 496.4 (5) \text{ \AA}^3$	$0.5 \times 0.4 \times 0.3 \text{ mm}$

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	2250 independent reflections
Radiation source: fine-focus sealed tube	2064 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.015$
$T = 293(2) \text{ K}$	$\theta_{\text{max}} = 28.3^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.5^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 9$
$T_{\text{min}} = 0.601$, $T_{\text{max}} = 0.721$	$k = -8 \rightarrow 11$
3041 measured reflections	$l = -12 \rightarrow 7$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H-atom parameters constrained
$wR(F^2) = 0.121$	$w = 1/[\sigma^2(F_o^2) + (0.0726P)^2 + 0.4272P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
2250 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
151 parameters	$\Delta\rho_{\text{max}} = 0.40 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.57 \text{ e \AA}^{-3}$
	Extinction correction: none

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.5000	1.0000	0.5000	0.02024 (16)
C1	0.6765 (4)	0.6477 (3)	-0.1760 (3)	0.0260 (5)
C2	0.6843 (4)	0.7807 (3)	-0.0285 (3)	0.0276 (6)
H2A	0.6609	0.8868	-0.0322	0.033*
C3	0.7249 (4)	0.7538 (3)	0.1145 (3)	0.0234 (5)

C4	0.7688 (4)	0.5932 (3)	0.1253 (3)	0.0241 (5)
C5	0.8169 (4)	0.5563 (4)	0.2709 (3)	0.0316 (6)
H5A	0.8186	0.6386	0.3666	0.038*
C6	0.8610 (5)	0.4004 (4)	0.2722 (4)	0.0363 (7)
H6A	0.8936	0.3779	0.3689	0.044*
C7	0.8573 (4)	0.2754 (4)	0.1295 (4)	0.0342 (6)
H7A	0.8882	0.1702	0.1320	0.041*
C8	0.8084 (4)	0.3057 (3)	-0.0152 (3)	0.0289 (6)
H8A	0.8052	0.2214	-0.1102	0.035*
C9	0.7636 (4)	0.4648 (3)	-0.0176 (3)	0.0233 (5)
C10	0.7168 (4)	0.8914 (3)	0.2641 (3)	0.0244 (5)
N1	0.7143 (3)	0.4972 (3)	-0.1615 (3)	0.0250 (5)
H1A	0.7072	0.4158	-0.2483	0.030*
O1	0.5726 (3)	0.8651 (3)	0.3072 (2)	0.0319 (5)
O2	0.8452 (3)	1.0169 (3)	0.3306 (3)	0.0337 (5)
O3	0.6381 (3)	0.6659 (3)	-0.3117 (2)	0.0342 (5)
O1W	0.2409 (3)	1.0448 (3)	0.3421 (3)	0.0331 (5)
H1	0.1249	1.0296	0.3471	0.050*
H2	0.2548	1.1369	0.3265	0.050*
O2W	0.3413 (3)	0.7783 (2)	0.4826 (2)	0.0274 (4)
H3	0.2601	0.8200	0.5308	0.041*
H4	0.4010	0.7217	0.5403	0.041*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0210 (3)	0.0197 (2)	0.0201 (2)	0.00347 (17)	0.01005 (17)	0.00379 (17)
C1	0.0249 (13)	0.0306 (14)	0.0230 (12)	0.0038 (10)	0.0085 (10)	0.0095 (11)
C2	0.0327 (14)	0.0266 (13)	0.0272 (13)	0.0085 (11)	0.0138 (11)	0.0103 (11)
C3	0.0207 (12)	0.0268 (13)	0.0229 (12)	0.0038 (10)	0.0106 (10)	0.0056 (10)
C4	0.0230 (12)	0.0274 (13)	0.0232 (12)	0.0039 (10)	0.0097 (10)	0.0085 (10)
C5	0.0353 (15)	0.0379 (16)	0.0218 (12)	0.0064 (12)	0.0103 (11)	0.0100 (11)
C6	0.0383 (16)	0.0423 (17)	0.0331 (15)	0.0042 (13)	0.0087 (12)	0.0226 (13)
C7	0.0323 (15)	0.0287 (14)	0.0425 (16)	0.0034 (11)	0.0071 (12)	0.0189 (13)
C8	0.0274 (13)	0.0241 (13)	0.0306 (13)	0.0029 (10)	0.0074 (11)	0.0059 (11)
C9	0.0196 (12)	0.0261 (13)	0.0237 (11)	0.0026 (10)	0.0070 (9)	0.0081 (10)
C10	0.0254 (13)	0.0264 (13)	0.0230 (12)	0.0083 (10)	0.0117 (10)	0.0070 (10)
N1	0.0294 (12)	0.0237 (11)	0.0191 (10)	0.0037 (9)	0.0089 (9)	0.0031 (8)
O1	0.0308 (10)	0.0314 (11)	0.0293 (10)	-0.0013 (8)	0.0176 (8)	-0.0020 (8)
O2	0.0316 (11)	0.0295 (11)	0.0388 (11)	-0.0002 (8)	0.0197 (9)	0.0026 (9)
O3	0.0412 (12)	0.0395 (12)	0.0251 (9)	0.0082 (9)	0.0111 (9)	0.0154 (9)
O1W	0.0257 (10)	0.0366 (11)	0.0390 (11)	0.0058 (8)	0.0100 (8)	0.0165 (9)
O2W	0.0304 (10)	0.0278 (10)	0.0263 (9)	0.0055 (8)	0.0127 (8)	0.0094 (8)

Geometric parameters (\AA , $^\circ$)

Ni1—O1 ⁱ	2.007 (2)	C5—H5A	0.9300
Ni1—O1	2.007 (2)	C6—C7	1.393 (5)

supplementary materials

Ni1—O1W	2.083 (2)	C6—H6A	0.9300
Ni1—O1W ⁱ	2.083 (2)	C7—C8	1.377 (4)
Ni1—O2W	2.117 (2)	C7—H7A	0.9300
Ni1—O2W ⁱ	2.117 (2)	C8—C9	1.401 (4)
C1—O3	1.254 (3)	C8—H8A	0.9300
C1—N1	1.351 (4)	C9—N1	1.379 (3)
C1—C2	1.447 (4)	C10—O2	1.244 (3)
C2—C3	1.352 (4)	C10—O1	1.250 (3)
C2—H2A	0.9300	N1—H1A	0.8600
C3—C4	1.433 (4)	O1W—H1	0.8501
C3—C10	1.514 (3)	O1W—H2	0.8500
C4—C9	1.405 (4)	O2W—H3	0.8500
C4—C5	1.414 (4)	O2W—H4	0.8499
C5—C6	1.371 (4)		
O1 ⁱ —Ni1—O1	180.0	C6—C5—H5A	119.7
O1 ⁱ —Ni1—O1W	90.69 (10)	C4—C5—H5A	119.7
O1—Ni1—O1W	89.31 (10)	C5—C6—C7	120.4 (3)
O1 ⁱ —Ni1—O1W ⁱ	89.31 (9)	C5—C6—H6A	119.8
O1—Ni1—O1W ⁱ	90.69 (10)	C7—C6—H6A	119.8
O1W—Ni1—O1W ⁱ	180.000 (1)	C8—C7—C6	120.8 (3)
O1 ⁱ —Ni1—O2W	91.65 (8)	C8—C7—H7A	119.6
O1—Ni1—O2W	88.35 (8)	C6—C7—H7A	119.6
O1W—Ni1—O2W	89.05 (9)	C7—C8—C9	119.2 (3)
O1W ⁱ —Ni1—O2W	90.95 (9)	C7—C8—H8A	120.4
O1 ⁱ —Ni1—O2W ⁱ	88.35 (8)	C9—C8—H8A	120.4
O1—Ni1—O2W ⁱ	91.65 (8)	N1—C9—C8	120.0 (2)
O1W—Ni1—O2W ⁱ	90.95 (9)	N1—C9—C4	119.1 (2)
O1W ⁱ —Ni1—O2W ⁱ	89.05 (9)	C8—C9—C4	120.9 (2)
O2W—Ni1—O2W ⁱ	180.00 (10)	O2—C10—O1	126.3 (2)
O3—C1—N1	120.0 (2)	O2—C10—C3	119.9 (2)
O3—C1—C2	123.8 (3)	O1—C10—C3	113.8 (2)
N1—C1—C2	116.2 (2)	C1—N1—C9	124.7 (2)
C3—C2—C1	121.4 (3)	C1—N1—H1A	117.6
C3—C2—H2A	119.3	C9—N1—H1A	117.6
C1—C2—H2A	119.3	C10—O1—Ni1	129.97 (18)
C2—C3—C4	120.6 (2)	Ni1—O1W—H1	123.7
C2—C3—C10	120.3 (2)	Ni1—O1W—H2	113.0
C4—C3—C10	119.0 (2)	H1—O1W—H2	109.1
C9—C4—C5	118.1 (3)	Ni1—O2W—H3	100.1
C9—C4—C3	117.9 (2)	Ni1—O2W—H4	118.4
C5—C4—C3	124.0 (2)	H3—O2W—H4	101.2
C6—C5—C4	120.6 (3)		
O3—C1—C2—C3	179.5 (3)	C5—C4—C9—C8	-1.2 (4)
N1—C1—C2—C3	-0.8 (4)	C3—C4—C9—C8	178.9 (2)
C1—C2—C3—C4	2.3 (4)	C2—C3—C10—O2	-69.5 (4)
C1—C2—C3—C10	-175.4 (2)	C4—C3—C10—O2	112.8 (3)

C2—C3—C4—C9	-1.4 (4)	C2—C3—C10—O1	109.5 (3)
C10—C3—C4—C9	176.2 (2)	C4—C3—C10—O1	-68.2 (3)
C2—C3—C4—C5	178.6 (3)	O3—C1—N1—C9	178.1 (2)
C10—C3—C4—C5	-3.7 (4)	C2—C1—N1—C9	-1.7 (4)
C9—C4—C5—C6	1.3 (4)	C8—C9—N1—C1	-177.2 (3)
C3—C4—C5—C6	-178.7 (3)	C4—C9—N1—C1	2.5 (4)
C4—C5—C6—C7	-0.6 (5)	O2—C10—O1—Ni1	-4.1 (4)
C5—C6—C7—C8	-0.3 (5)	C3—C10—O1—Ni1	176.92 (17)
C6—C7—C8—C9	0.5 (4)	O1W—Ni1—O1—C10	115.2 (3)
C7—C8—C9—N1	-180.0 (2)	O1W ⁱ —Ni1—O1—C10	-64.8 (3)
C7—C8—C9—C4	0.3 (4)	O2W—Ni1—O1—C10	-155.7 (3)
C5—C4—C9—N1	179.1 (2)	O2W ⁱ —Ni1—O1—C10	24.3 (3)
C3—C4—C9—N1	-0.9 (4)		

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

Hydrogen-bond 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>
N1—H1A...O2W ⁱⁱ	0.86	2.18	3.031 (3)	173
O1W—H1...O2 ⁱⁱⁱ	0.85	1.94	2.783 (3)	169
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Symmetry codes: (ii) $-x+1, -y+1, -z$; (iii) $x-1, y, z$; (iv) $-x+1, -y+2, -z$; (i) $-x+1, -y+2, -z+1$; (v) $x, y, z+1$.

Fig. 1

