Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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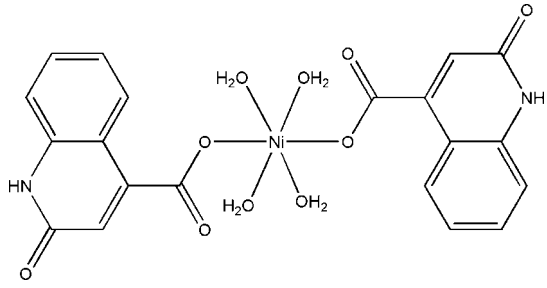
Received 13 November 2007; accepted 5 December 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(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···O and N—H···O) and offset face-to-face π–π 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, $P\overline{1}$
a = 7.105 (5) Å
b = 8.507 (5) Å
c = 9.216 (5) Å
α = 108.723 (5)°
β = 108.396 (5)°
γ = 90.840 (5)°
V = 496.4 (5) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.04 mm^{-1}
T = 293 (2) K
0.5 × 0.4 × 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—O2*W*	2.117 (2)
Ni1—O1*W*	2.083 (2)		
O1—Ni1—O1*W*	89.31 (10)	O1*W*—Ni1—O2*W*	89.05 (9)
O1—Ni1—O1*W*^{i}	90.69 (10)	O1*W*^{i}—Ni1—O2*W*	90.95 (9)
O1—Ni1—O2*W*	88.35 (8)	O1—Ni1—O2*W*^{i}	91.65 (8)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2*W*^{ii}	0.86	2.18	3.031 (3)	173
O1*W*—H1···O2^{iii}	0.85	1.94	2.783 (3)	169
O1*W*—H2···O3^{iv}	0.85	1.89	2.722 (3)	164
O2*W*—H3···O2^{i}	0.85	1.90	2.709 (3)	158
O2*W*—H4···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*.

We thank the Changjiang Scholars and Innovative Research Team in Universities Program, the National Natural Science Foundation of China (grant No. 20573016) and the Science Foundation for Young Teachers of Northeast Normal University (grant No. 20070310) for financial support.

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). E**64**, m389-m390 [**doi:10.1107/S1600536807065671**]

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

G. Yuan, J.-S. Qin, Z.-M. Su, K.-Z. Shao and Y.-M. Fu

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-hydroquinoline-4-carboxylic acid (hqc) and $NiCl_2$ 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···O and N–H···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 $NiCl_2.6H_2O$ (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 = 0.86Å and U_{iso}(H)=1.2U_{eq}(C,*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_{iso}(H)=1.5U_{eq}(O).

Figures

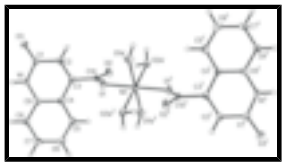


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) 1 - *x*, 2 - *y*, 1 - *z*.]

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

Crystal data

$[Ni(C_{10}H_6NO_3)_2(H_2O)_4]$ $Z = 1$

M_r = 507.07	F_{000} = 262
Triclinic, $P\bar{1}$	D_x = 1.696 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71069 Å
a = 7.105 (5) Å	Cell parameters from 2250 reflections
b = 8.507 (5) Å	θ = 1.3–26.0º
c = 9.216 (5) Å	μ = 1.04 mm^{-1}
α = 108.723 (5)º	T = 293 (2) K
β = 108.396 (5)º	Block, green
γ = 90.840 (5)º	0.5 × 0.4 × 0.3 mm
V = 496.4 (5) Å^3	

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_{int} = 0.015
T = 293(2) K	θ_{max} = 28.3º
φ and ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −9→9
T_{min} = 0.601, T_{max} = 0.721	k = −8→11
3041 measured reflections	l = −12→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	$w = 1/[\sigma^2(F_o^2) + (0.0726P)^2 + 0.4272P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
2250 reflections	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
151 parameters	$\Delta\rho_{min}$ = −0.57 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	y	z	U_{iso}*/U_{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 (Å^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 (Å, °)

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

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)		

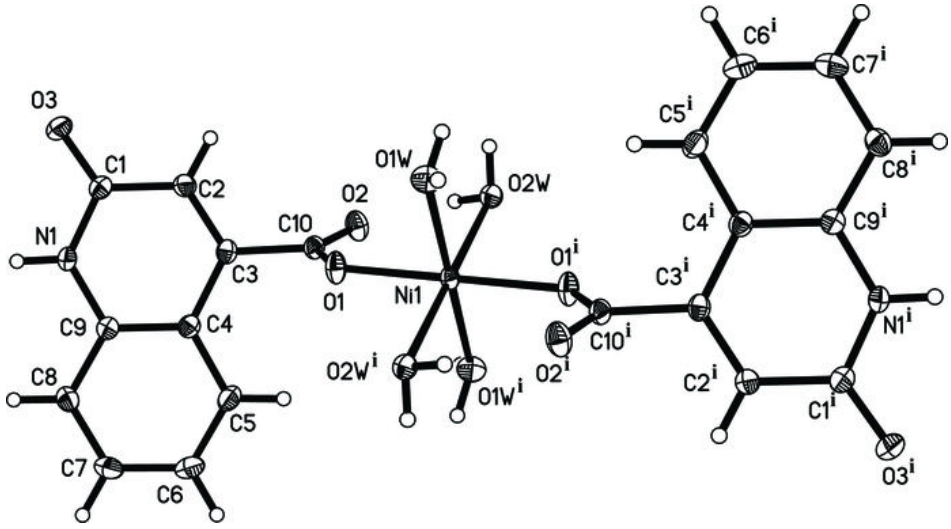
Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1.

Hydrogen-bond geometry (Å, °)

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

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


O3
C1
C2
N1
C10
O2
C3
O1
Ni1
O1W
O2W
C9
C4
C8
C5
C7
C6
O2W^{i}
O1W^{i}
O1^{i}
C10^{i}
O2^{i}
C6^{i}
C7^{i}
C5^{i}
C8^{i}
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N1^{i}
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O3^{i}