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trans-Diaquabis(quinoline-2-carboxylato-*N*,*O*)-nickel(II)–water–ethanol (1/2/2)

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The title compound, $[Ni(C_{10}H_6NO_2)_2(H_2O)_2]\cdot2H_2O\cdot2C_2H_5OH$, contains a six-coordinate Ni^{II} ion displaying distorted octahedral coordination geometry defined by the two quinoline N atoms, two O atoms of the carboxylate groups and two O atoms of the water molecules. All of the corresponding pairs of ligand atoms lie in *trans* positions with respect to each other, the Ni atom lying on an inversion center. Molecules are linked together by an intermolecular hydrogen-bonding network involving the uncoordinated water and ethanol molecules.

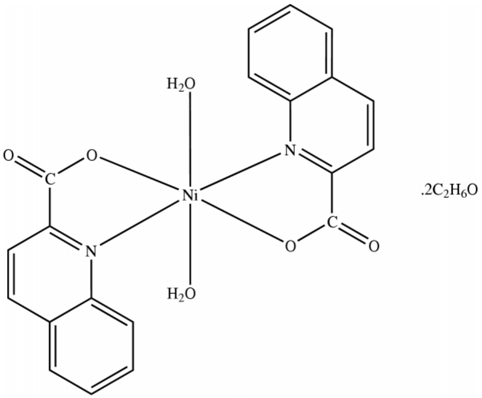
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.033
wR factor = 0.118
Data-to-parameter ratio = 16.8

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

Comment

2-Quinolinecarboxylic acid is an intermediate of tryptophan metabolism and is known to chelate transition metal ions (Martell & Smith, 1974). Crystal structures of metal complexes of 2-quinolinecarboxylic acid have been determined for several metal ions, including Cu^{II} (Haendler, 1986), Mn^{II} (Haendler, 1996; Okabe & Koizumi, 1997), Fe^{II} and Co^{II} (Okabe & Makino, 1998, 1999). We have obtained crystals of the title compound, (I), and carried out the structural analysis of the Ni^{II} complex.



(I)

The Ni^{II} complex is hexacoordinate with the Ni^{II} ion at a center of symmetry, similar to Mn^{II}, Fe^{II} and Co^{II} complexes. The two 2-quinolinecarboxylate ligands chelate the metal through the N atom and one O atom to form the equatorial plane. Two water molecules are located at the axial position and complete the octahedron. The 2-quinolinecarboxylate and the Ni^{II} ion form a five-membered ring, which is also present in the other complexes. In this ring, the Ni—O bonds are 2.013 (2) Å and Ni—N bonds are 2.185 (2) Å. Therefore, the metal—O and the metal—N bond lengths decrease in the order Mn > Fe > Co > Ni > Cu. Two uncoordinated water

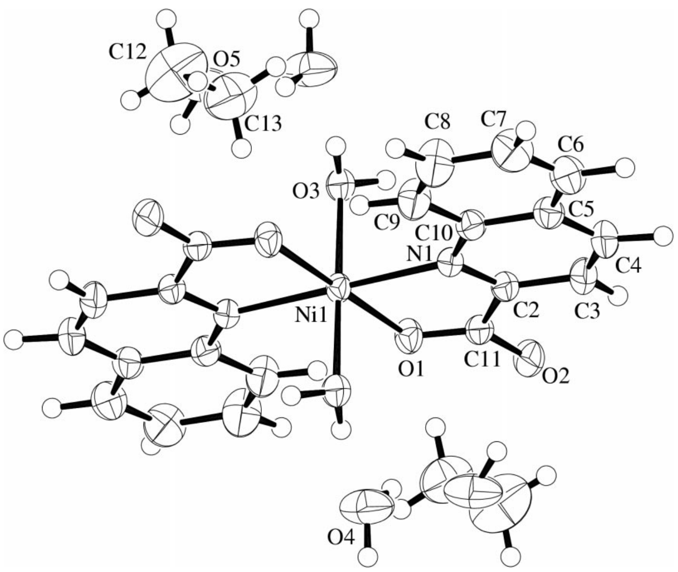


Figure 1
*ORTEP*II (Johnson, 1976) drawing of the title compound. Ellipsoids for non-H atoms are shown at the 50% probability level.

molecules and two uncoordinated ethanol molecules per molecule of complex are present in this structure. Similar water and ethanol molecules are found in the Mn, Fe and Co complexes. These molecules are linked together by a hydrogen-bonding network involving the complex molecules, uncoordinated water and ethanol molecules.

Experimental

Light-blue pillar-shaped crystals of the title compound were obtained at room temperature by the slow evaporation of a mixture of an ethanol–water solution (*ca* 50%) of 2-quinolinecarboxylic acid and nickel(II) acetate tetrahydrate (molar ratio 4:1).

Crystal data

$[Ni(C_{10}H_6NO_2)_2(H_2O)_2]\cdot 2C_2H_6O\cdot 2H_2O$
$M_r = 567.21$
Triclinic, $P\overline{1}$
$a = 8.978\ (1)$ Å
$b = 11.073\ (2)$ Å
$c = 7.2349\ (7)$ Å
$\alpha = 106.250\ (10)^\circ$
$\beta = 107.399\ (9)^\circ$
$\gamma = 78.47\ (1)^\circ$
$V = 653.6\ (1)$ Å^3
$Z = 1$
$D_x = 1.441$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 14.9$–15.0°
$\mu = 0.80$ mm^{-1}
$T = 296.2$ K
Pillar, light blue
0.4 × 0.2 × 0.1 mm

Data collection

Rigaku AFC-5*R* diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.822$, $T_{max} = 0.923$
3199 measured reflections
3010 independent reflections
2838 reflections with $I > 2\sigma(I)$
$R_{int} = 0.008$
$\theta_{max} = 27.5^\circ$
$h = 0 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -9 \rightarrow 8$
3 standard reflections every 150 reflections intensity decay: 1.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.118$
$S = 1.03$
2838 reflections
169 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = -0.003$
$\Delta\rho_{max} = 0.80$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	2.013 (2)	C3—C4	1.362 (3)
Ni1—O3	2.082 (1)	C4—C5	1.407 (4)
Ni1—N1	2.185 (2)	C5—C6	1.419 (3)
O1—C11	1.255 (3)	C5—C10	1.420 (3)
O2—C11	1.247 (3)	C6—C7	1.358 (4)
O5—C13	1.412 (4)	C7—C8	1.407 (4)
N1—C2	1.323 (3)	C8—C9	1.370 (3)
N1—C10	1.375 (2)	C9—C10	1.411 (4)
C2—C3	1.406 (3)	C12—C13	1.444 (7)
C2—C11	1.510 (2)		
O1—Ni1—O3	90.84 (5)	C4—C5—C10	118.3 (2)
O1—Ni1—N1	78.53 (6)	C6—C5—C10	119.6 (2)
O3—Ni1—N1	90.07 (6)	C5—C6—C7	120.4 (2)
Ni1—O1—C11	118.1 (1)	C6—C7—C8	119.7 (2)
Ni1—N1—C2	110.3 (1)	C7—C8—C9	121.8 (3)
Ni1—N1—C10	131.7 (1)	C8—C9—C10	119.6 (2)
C2—N1—C10	117.9 (2)	N1—C10—C5	121.4 (2)
N1—C2—C3	123.9 (2)	N1—C10—C9	119.7 (2)
N1—C2—C11	115.9 (2)	C5—C10—C9	118.9 (2)
C3—C2—C11	120.2 (2)	O1—C11—O2	124.4 (2)
C2—C3—C4	118.9 (2)	O1—C11—C2	117.1 (2)
C3—C4—C5	119.5 (2)	O2—C11—C2	118.5 (2)
C4—C5—C6	122.1 (2)	O5—C13—C12	113.2 (4)
Ni1—O1—C11—O2	178.5 (1)	O3—Ni1—N1^{i}—C2^{i}	−92.2 (1)
Ni1—O1—C11—C2	0.6 (2)	O3—Ni1—N1^{i}—C10^{i}	89.4 (1)
Ni1—O1^{i}—C11^{i}—O2^{i}	−178.5 (1)	N1—Ni1—O1—C11	−2.0 (1)
Ni1—O1^{i}—C11^{i}—C2^{i}	−0.6 (2)	N1—Ni1—O1^{i}—C11^{i}	−178.0 (1)
Ni1—N1—C2—C3	177.6 (1)	N1—C2—C3—C4	1.2 (3)
Ni1—N1—C2—C11	−3.7 (2)	N1—C10—C5—C4	0.5 (2)
Ni1—N1—C10—C5	−178.1 (1)	N1—C10—C5—C6	−179.3 (2)
Ni1—N1—C10—C9	3.1 (2)	N1—C10—C9—C8	179.3 (2)
Ni1—N1^{i}—C2^{i}—C3^{i}	−177.6 (1)	C2—N1—C10—C5	0.2 (2)
Ni1—N1^{i}—C2^{i}—C11^{i}	3.7 (2)	C2—N1—C10—C9	−178.6 (2)
Ni1—N1^{i}—C10^{i}—C5^{i}	178.1 (1)	C2—C3—C4—C5	−0.3 (3)
Ni1—N1^{i}—C10^{i}—C9^{i}	−3.1 (2)	C3—C2—N1—C10	−1.1 (2)
O1—Ni1—N1—C2	3.1 (1)	C3—C4—C5—C6	179.3 (2)
O1—Ni1—N1—C10	−178.5 (1)	C3—C4—C5—C10	−0.5 (3)
O1—Ni1—N1^{i}—C2^{i}	176.9 (1)	C4—C3—C2—C11	−177.6 (2)
O1—Ni1—N1^{i}—C10^{i}	−1.5 (1)	C4—C5—C6—C7	−179.8 (2)
O1—C11—C2—N1	2.3 (2)	C4—C5—C10—C9	179.4 (2)
O1—C11—C2—C3	−178.8 (2)	C5—C6—C7—C8	0.3 (3)
O2—C11—C2—N1	−175.7 (1)	C5—C10—C9—C8	0.5 (3)
O2—C11—C2—C3	3.1 (2)	C6—C5—C10—C9	−0.4 (3)
O3—Ni1—O1—C11	88.0 (1)	C6—C7—C8—C9	−0.3 (4)
O3—Ni1—O1^{i}—C11^{i}	92.0 (1)	C7—C6—C5—C10	0.0 (3)
O3—Ni1—N1—C2	−87.8 (1)	C7—C8—C9—C10	−0.1 (3)
O3—Ni1—N1—C10	90.6 (1)	C10—N1—C2—C11	177.7 (1)

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

H atoms were placed in calculated ideal positions, with the exception of those involved in hydrogen bonding, which were located in a difference Fourier map and were not refined.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *teXsan* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999) and *DIRDIF*94 (Beurskens *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *teXsan*.

m268 Mamiko Odoko *et al.* • $[Ni(C_{10}H_6NO_2)_2(H_2O)_2]\cdot 2C_2H_6O\cdot 2H_2O$ *Acta Cryst.* (2001). E**57**, m267–m269

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