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Diaquabis[4-(4*H*-1,2,4-triazol-4-yl)-benzoato-κ^2O,O']nickel(II)

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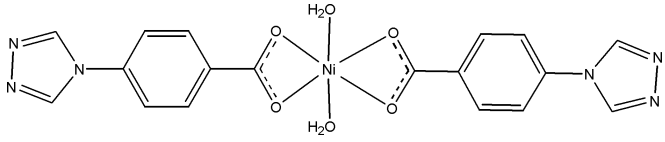
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.084; data-to-parameter ratio = 11.9.

In the title compound, $[Ni(C_9H_6N_3O_2)_2(H_2O)_2]$, the Ni^{II} atom lies on a twofold rotation axis and is six-coordinated by two bidentate chelating 4-(1,2,4-triazol-4-yl)benzoate ligands and two water molecules in a distorted octahedral geometry. Intermolecular O—H···N hydrogen bonds link the complex molecules into a two-dimensional network parallel to (010).

Related literature

For general background to the structures and applications of metal complexes, see: Mahata *et al.* (2009); Perry *et al.* (2004); Qin *et al.* (2005); Shi *et al.* (2009). For a related structure, see: Zhu (2010).



Experimental

Crystal data

$[Ni(C_9H_6N_3O_2)_2(H_2O)_2]$
M_r = 471.06
Monoclinic, $C2/c$
a = 13.5194 (6) Å
b = 9.8480 (5) Å
c = 14.3234 (7) Å
β = 112.293 (1)°
V = 1764.47 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.16 mm^{-1}
T = 296 K
0.28 × 0.24 × 0.22 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.72, T_{max} = 0.82
4732 measured reflections
1744 independent reflections
1662 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.084
S = 1.13
1744 reflections
147 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—O1	2.1507 (14)	Ni1—O3	2.0453 (16)
Ni1—O2	2.1240 (14)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3B···N2^{i}	0.78 (2)	2.06 (2)	2.836 (2)	172 (3)
O3—H3A···N3^{ii}	0.79 (2)	1.99 (2)	2.768 (2)	169 (3)

Symmetry codes: (i) $-x, y, -z+\frac{3}{2}$; (ii) $x+1, -y, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2427).

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supporting information

Acta Cryst. (2011). E**67**, m728 [doi:10.1107/S1600536811016643]

Diaquabis[4-(4*H*-1,2,4-triazol-4-yl)benzoato-κ^2O,O']nickel(II)

Shuzhi Xu, Wenxin Shao, Miao Yu and Guihua Gong

S1. Comment

The construction of novel coordination complexes is the current interest in the field of supramolecular chemistry and crystal engineering stemming from their potential applications as functional materials, as well as their intriguing variety of architectures and topologies (Perry *et al.*, 2004; Qin *et al.*, 2005). Heterocyclic carboxylates have often been used as mono-, bi- or multi-dentate ligands to bind transition metal centers, leading to the formation of moderately robust metal–organic coordination frameworks (Mahata *et al.*, 2009; Shi *et al.*, 2009). In this contribution, we selected 4-(1,2,4-triazol-4-yl)benzoic acid (Htyb) as an organic carboxylate ligand, generating the title compound, which is reported here.

In the title compound, the Ni^{II} atom lies on a twofold rotation axis and adopts a distorted octahedral coordination geometry, being coordinated by four carboxylate O atoms from two tyb ligands and two water molecules (Fig. 1, Table 1). The Ni—O bond lengths and the O—Ni—O bond angles are in the normal range (Zhu, 2010). Intermolecular O—H···N hydrogen bonds (Table 2) stabilize the structure and give a two-dimensional network (Fig. 2).

S2. Experimental

The synthesis was performed under hydrothermal conditions. A mixture of $Ni(CH_3COO)_2.4H_2O$ (0.2 mmol, 0.05 g), 4-(1,2,4-triazol-4-yl)benzoic acid (0.4 mmol, 0.075 g), NaOH (0.4 mmol, 0.016 g) and H_2O (15 ml) in a 25 ml stainless steel reactor with a Teflon liner was heated from 293 to 443 K in 2 h and a constant temperature was maintained at 443 K for 72 h. After the mixture was cooled to 298 K, green crystals of the title compound were obtained.

S3. Refinement

H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C). H atoms bonded to water O atom were located in a difference Fourier map and refined with a restraint of O—H = 0.85 (1) Å.

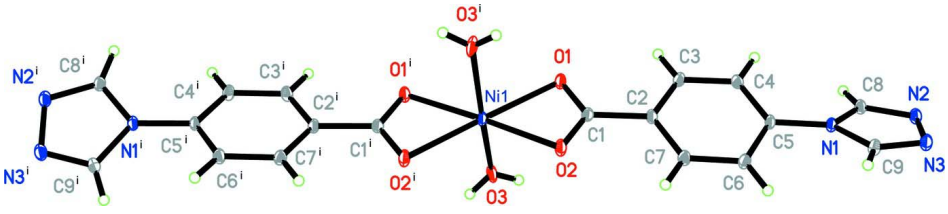

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) 1-*x*, *y*, 3/2-*z*.]

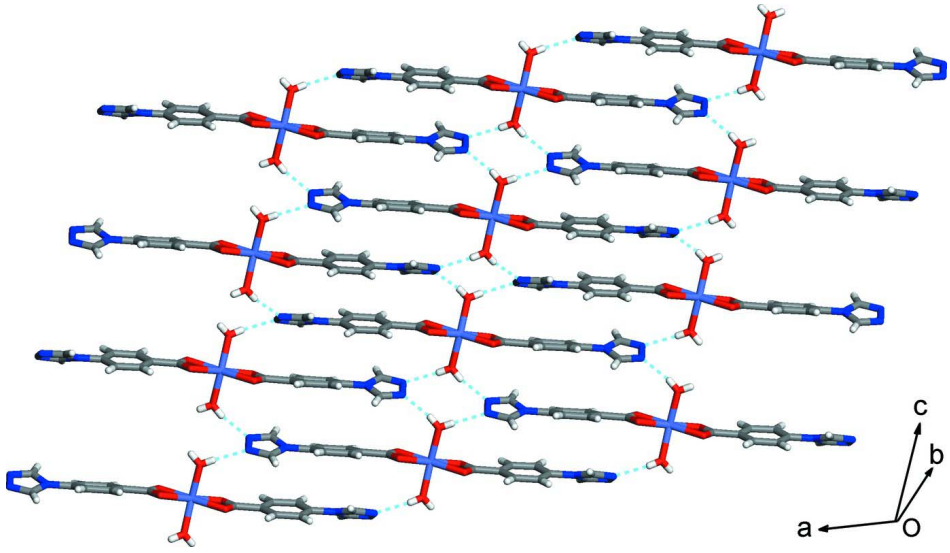

Figure 2

View of the layer structure in the title compound, built by O—H···N hydrogen bonds (dashed lines).

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$c = 14.3234\ (7)$ Å
$\beta = 112.293\ (1)°$
$V = 1764.47\ (15)$ Å^3
$Z = 4$
$F(000) = 968$
$D_x = 1.773$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1744 reflections
$\theta = 1.0–26.0°$
$\mu = 1.16$ mm^{-1}
$T = 296$ K
Block, green
0.28 × 0.24 × 0.22 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.72$, $T_{max} = 0.82$
4732 measured reflections
1744 independent reflections
1662 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.6°$
$h = -16\rightarrow16$
$k = -12\rightarrow9$
$l = -14\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.084$
$S = 1.13$
1744 reflections
147 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 4.2534P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.30391 (16)	0.07262 (19)	0.68990 (15)	0.0139 (4)
C2	0.18541 (15)	0.0695 (2)	0.66363 (15)	0.0144 (4)
C3	0.12703 (16)	0.1900 (2)	0.64420 (15)	0.0164 (4)
H3	0.1616	0.2723	0.6465	0.020*
C4	0.01757 (15)	0.1882 (2)	0.62145 (15)	0.0164 (4)
H4	−0.0217	0.2684	0.6074	0.020*
C5	−0.03212 (15)	0.0645 (2)	0.62014 (15)	0.0132 (4)
C6	0.02504 (16)	−0.0562 (2)	0.64143 (16)	0.0167 (4)
H6	−0.0092	−0.1381	0.6416	0.020*
C7	0.13424 (16)	−0.0531 (2)	0.66248 (16)	0.0163 (4)
H7	0.1732	−0.1336	0.6759	0.020*
C8	−0.21097 (15)	0.1595 (2)	0.60494 (15)	0.0157 (4)
H8	−0.1890	0.2466	0.6290	0.019*
C9	−0.21064 (16)	−0.0489 (2)	0.55868 (16)	0.0178 (4)
H9	−0.1883	−0.1332	0.5450	0.021*
N1	−0.14499 (13)	0.05953 (17)	0.59661 (12)	0.0136 (4)
N2	−0.30914 (13)	0.11583 (19)	0.57442 (13)	0.0176 (4)
N3	−0.30856 (13)	−0.01823 (19)	0.54433 (13)	0.0188 (4)
O1	0.35080 (11)	0.18546 (14)	0.69937 (11)	0.0162 (3)
O2	0.35618 (11)	−0.03741 (15)	0.70360 (11)	0.0184 (3)
O3	0.50303 (12)	0.10080 (19)	0.89291 (12)	0.0248 (4)
Ni1	0.5000	0.07701 (4)	0.7500	0.01674 (14)
H3A	0.5529 (17)	0.080 (3)	0.9416 (16)	0.025*
H3B	0.4511 (17)	0.113 (3)	0.903 (2)	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0112 (10)	0.0169 (10)	0.0139 (9)	−0.0001 (7)	0.0050 (8)	−0.0002 (7)
C2	0.0097 (10)	0.0186 (10)	0.0148 (9)	0.0000 (7)	0.0045 (8)	−0.0001 (7)
C3	0.0125 (9)	0.0150 (10)	0.0218 (10)	−0.0022 (8)	0.0066 (8)	0.0014 (8)
C4	0.0114 (9)	0.0149 (10)	0.0221 (10)	0.0024 (7)	0.0056 (8)	0.0033 (8)
C5	0.0073 (9)	0.0189 (10)	0.0132 (9)	−0.0003 (7)	0.0038 (7)	−0.0006 (7)
C6	0.0122 (10)	0.0153 (10)	0.0229 (11)	−0.0022 (8)	0.0069 (8)	−0.0005 (8)
C7	0.0124 (10)	0.0142 (9)	0.0229 (10)	0.0018 (8)	0.0075 (8)	0.0003 (8)
C8	0.0104 (9)	0.0193 (10)	0.0174 (10)	0.0019 (8)	0.0053 (8)	0.0006 (8)
C9	0.0135 (10)	0.0188 (10)	0.0204 (10)	−0.0034 (8)	0.0056 (8)	−0.0026 (8)
N1	0.0087 (8)	0.0164 (8)	0.0156 (8)	−0.0013 (6)	0.0045 (7)	−0.0001 (6)
N2	0.0110 (8)	0.0230 (9)	0.0183 (9)	−0.0001 (7)	0.0049 (7)	0.0005 (7)
N3	0.0118 (8)	0.0232 (9)	0.0203 (9)	−0.0025 (7)	0.0047 (7)	−0.0003 (7)
O1	0.0089 (6)	0.0161 (7)	0.0231 (7)	−0.0010 (5)	0.0054 (6)	0.0001 (6)

O2	0.0091 (6)	0.0164 (7)	0.0293 (8)	0.0008 (6)	0.0070 (6)	0.0005 (6)
O3	0.0090 (7)	0.0468 (10)	0.0188 (8)	0.0075 (7)	0.0054 (6)	0.0057 (7)
Ni1	0.0100 (2)	0.0175 (2)	0.0222 (2)	0.000	0.00558 (16)	0.000

Geometric parameters (Å, º)

C1—O1	1.261 (2)	C7—H7	0.9300
C1—O2	1.268 (2)	C8—N2	1.303 (3)
C1—C2	1.501 (3)	C8—N1	1.364 (3)
C1—Ni1	2.458 (2)	C8—H8	0.9300
C2—C7	1.388 (3)	C9—N3	1.296 (3)
C2—C3	1.394 (3)	C9—N1	1.363 (3)
C3—C4	1.389 (3)	C9—H9	0.9300
C3—H3	0.9300	N2—N3	1.390 (3)
C4—C5	1.388 (3)	O3—H3A	0.79 (2)
C4—H4	0.9300	O3—H3B	0.78 (2)
C5—C6	1.387 (3)	Ni1—O1	2.1507 (14)
C5—N1	1.433 (2)	Ni1—O2	2.1240 (14)
C6—C7	1.391 (3)	Ni1—O3	2.0453 (16)
C6—H6	0.9300		
O1—C1—O2	120.58 (18)	C9—N3—N2	107.32 (17)
O1—C1—C2	119.38 (17)	C1—O1—Ni1	88.14 (11)
O2—C1—C2	120.03 (17)	C1—O2—Ni1	89.16 (12)
O1—C1—Ni1	61.01 (10)	Ni1—O3—H3A	123 (2)
O2—C1—Ni1	59.79 (10)	Ni1—O3—H3B	122 (2)
C2—C1—Ni1	174.50 (14)	H3A—O3—H3B	114 (3)
C7—C2—C3	119.77 (18)	O3—Ni1—O3^{i}	166.84 (11)
C7—C2—C1	120.05 (18)	O3—Ni1—O2	92.43 (6)
C3—C2—C1	120.14 (17)	O3^{i}—Ni1—O2	94.54 (6)
C4—C3—C2	120.52 (18)	O3—Ni1—O2^{i}	94.54 (6)
C4—C3—H3	119.7	O3^{i}—Ni1—O2^{i}	92.43 (6)
C2—C3—H3	119.7	O2—Ni1—O2^{i}	115.92 (8)
C5—C4—C3	118.77 (18)	O3—Ni1—O1^{i}	86.88 (6)
C5—C4—H4	120.6	O3^{i}—Ni1—O1^{i}	86.60 (6)
C3—C4—H4	120.6	O2—Ni1—O1^{i}	177.55 (6)
C6—C5—C4	121.53 (18)	O2^{i}—Ni1—O1^{i}	61.82 (6)
C6—C5—N1	118.50 (17)	O3—Ni1—O1	86.60 (6)
C4—C5—N1	119.97 (17)	O3^{i}—Ni1—O1	86.88 (6)
C5—C6—C7	119.07 (18)	O2—Ni1—O1	61.82 (6)
C5—C6—H6	120.5	O2^{i}—Ni1—O1	177.55 (6)
C7—C6—H6	120.5	O1^{i}—Ni1—O1	120.45 (8)
C2—C7—C6	120.32 (19)	O3—Ni1—C1	87.82 (6)
C2—C7—H7	119.8	O3^{i}—Ni1—C1	92.41 (6)
C6—C7—H7	119.8	O2—Ni1—C1	31.05 (6)
N2—C8—N1	110.45 (18)	O2^{i}—Ni1—C1	146.94 (6)
N2—C8—H8	124.8	O1^{i}—Ni1—C1	151.16 (6)
N1—C8—H8	124.8	O1—Ni1—C1	30.85 (6)

N3—C9—N1	110.64 (19)	O3—Ni1—C1^{i}	92.41 (6)
N3—C9—H9	124.7	O3^{i}—Ni1—C1^{i}	87.82 (6)
N1—C9—H9	124.7	O2—Ni1—C1^{i}	146.94 (6)
C9—N1—C8	104.57 (17)	O2^{i}—Ni1—C1^{i}	31.05 (6)
C9—N1—C5	126.49 (17)	O1^{i}—Ni1—C1^{i}	30.85 (6)
C8—N1—C5	128.93 (17)	O1—Ni1—C1^{i}	151.16 (6)
C8—N2—N3	107.02 (16)	C1—Ni1—C1^{i}	177.99 (9)
O1—C1—C2—C7	−173.79 (19)	N1—C9—N3—N2	−0.5 (2)
O2—C1—C2—C7	5.3 (3)	C8—N2—N3—C9	0.4 (2)
O1—C1—C2—C3	3.7 (3)	O2—C1—O1—Ni1	−5.41 (19)
O2—C1—C2—C3	−177.18 (18)	C2—C1—O1—Ni1	173.72 (16)
C7—C2—C3—C4	−1.4 (3)	O1—C1—O2—Ni1	5.47 (19)
C1—C2—C3—C4	−178.94 (18)	C2—C1—O2—Ni1	−173.65 (16)
C2—C3—C4—C5	1.1 (3)	C1—O2—Ni1—O3	81.70 (12)
C3—C4—C5—C6	0.3 (3)	C1—O2—Ni1—O3^{i}	−87.13 (12)
C3—C4—C5—N1	−179.81 (17)	C1—O2—Ni1—O2^{i}	177.95 (13)
C4—C5—C6—C7	−1.4 (3)	C1—O1—Ni1—O3	−91.44 (12)
N1—C5—C6—C7	178.78 (18)	C1—O1—Ni1—O3^{i}	100.00 (12)
C3—C2—C7—C6	0.4 (3)	C1—O1—Ni1—O2	3.15 (11)
C1—C2—C7—C6	177.89 (18)	C1—O1—Ni1—O1^{i}	−175.80 (12)
C5—C6—C7—C2	1.0 (3)	O1—C1—Ni1—O3	87.02 (12)
N3—C9—N1—C8	0.4 (2)	O2—C1—Ni1—O3	−98.36 (12)
N3—C9—N1—C5	−178.76 (17)	O1—C1—Ni1—O3^{i}	−79.81 (12)
N2—C8—N1—C9	−0.1 (2)	O2—C1—Ni1—O3^{i}	94.80 (12)
N2—C8—N1—C5	178.99 (18)	O1—C1—Ni1—O2	−174.61 (19)
C6—C5—N1—C9	−24.4 (3)	O1—C1—Ni1—O2^{i}	−178.00 (10)
C4—C5—N1—C9	155.7 (2)	O2—C1—Ni1—O2^{i}	−3.4 (2)
C6—C5—N1—C8	156.7 (2)	O1—C1—Ni1—O1^{i}	7.5 (2)
C4—C5—N1—C8	−23.2 (3)	O2—C1—Ni1—O1^{i}	−177.86 (11)
N1—C8—N2—N3	−0.2 (2)	O2—C1—Ni1—O1	174.61 (19)

Symmetry code: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*B*···N2^{ii}	0.78 (2)	2.06 (2)	2.836 (2)	172 (3)
O3—H3*A*···N3^{iii}	0.79 (2)	1.99 (2)	2.768 (2)	169 (3)

Symmetry codes: (ii) −*x*, *y*, −*z*+3/2; (iii) *x*+1, −*y*, *z*+1/2.