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Tetraaquabis[3-(4-pyridyl)benzoato-κN]-nickel(II)

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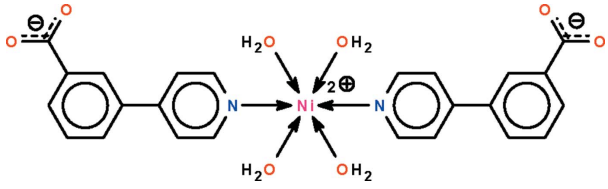
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.090; data-to-parameter ratio = 13.5.

The Ni^{II} atom in the title compound, $[Ni(C_{12}H_8NO_2)_2(H_2O)_4]$, exists in an all-*trans* octahedral coordination environment. The 3-(4-pyridyl)benzoate ligand binds to Ni atom through the pyridyl N atom; the pyridine and benzene rings are oriented at a dihedral angle of 26.27 (10)°. Adjacent complexes are linked by O—H···O hydrogen bonds, forming a three-dimensional network. The metal atom lies on a special position of 2 site symmetry in the crystal structure.

Related literature

The 3-(pyridin-4-yl)benzoate unit is fairly rigid like the nicotinate unit, which also forms a similar zwitterionic nickel derivative; see: Batten & Harris (2001).



Experimental

Crystal data

$[Ni(C_{12}H_8NO_2)_2(H_2O)_4]$
M_r = 527.16
Monoclinic, $C2/c$
a = 24.564 (3) Å
b = 7.0520 (8) Å
c = 13.781 (2) Å
β = 113.325 (2)°
V = 2192.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.94 mm^{-1}
T = 173 K
0.47 × 0.31 × 0.08 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.666, T_{max} = 0.929
5587 measured reflections
2360 independent reflections
1977 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.090
S = 1.09
2360 reflections
175 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—O1W	2.0627 (14)	Ni1—N1	2.0931 (16)
Ni1—O2W	2.0811 (14)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H11···O1^{i}	0.84 (1)	1.88 (1)	2.682 (2)	160 (3)
O1w—H12···O2^{ii}	0.83 (1)	1.91 (1)	2.734 (2)	170 (2)
O2w—H21···O1^{iii}	0.84 (1)	1.93 (1)	2.732 (2)	159 (2)
O2w—H22···O2^{iv}	0.83 (1)	1.88 (1)	2.711 (2)	177 (3)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2699).

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supplementary materials

Acta Cryst. (2009). E**65**, m1708 [**doi:10.1107/S1600536809051204**]

Tetraaquabis[3-(4-pyridyl)benzoato-*κN*]nickel(II)

Q.-X. Wang, M.-H. Zeng and S. W. Ng

Experimental

3-(Pyridin-4-yl)benzoic acid was purchased from a chemical supplier. The reagent (0.199 g, 1 mmol) and sodium hydroxide (0.040 g, 1 mmol) were mixed with nickel(II) nitrate hexahydrate (0.150 g, 0.5 mmol) in water (10 ml). The mixture was placed in a 15 ml Teflon-lined autoclave and heated at 423 K for 48 h. The autoclave was cooled over 12 h at a rate of 5 K an hour. Green crystals were isolated by hand (yield *ca* 60% based on Ni).

Refinement

Carbon-bound hydrogen atoms were generated geometrically and were constrained to ride on their parent atoms [C–H = 0.95 Å; U_{iso}(H) =1.2U_{eq}(C)]. The water H-atoms were located in a difference Fourier map, and were refined with a distance restraint of O–H 0.84±0.01 Å; their temperature factors were refined.

Figures

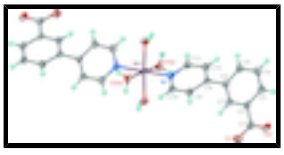

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $Ni(H_2O)_4(C_{12}H_2NO_2)_2$ at the 70% probability level; hydrogen atoms are drawn as sphere of arbitrary radius.

Tetraaquabis[3-(4-pyridyl)benzoato-κ*N*]nickel(II)

Crystal data

$[Ni(C_{12}H_8NO_2)_2(H_2O)_4]$	$F(000)$ = 1096
M_r = 527.16	D_x = 1.597 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 996 reflections
a = 24.564 (3) Å	θ = 3.0–26.9°
b = 7.0520 (8) Å	μ = 0.94 mm^{-1}
c = 13.781 (2) Å	*T* = 173 K
β = 113.325 (2)°	Prism, green
V = 2192.1 (4) Å^3	0.47 × 0.31 × 0.08 mm
Z = 4	

Data collection

Bruker APEXII diffractometer	2360 independent reflections

Radiation source: fine-focus sealed tube	1977 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.023$
φ and ω scans	$\theta_{max} = 27.0°$, $\theta_{min} = 1.8°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -10 \rightarrow 31$
$T_{min} = 0.666$, $T_{max} = 0.929$	$k = -8 \rightarrow 8$
5587 measured reflections	$l = -17 \rightarrow 10$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.031$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.090$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.09$	$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.5684P]$ where $P = (F_o^2 + 2F_c^2)/3$
2360 reflections	$(\Delta/\sigma)_{max} = 0.001$
175 parameters	$\Delta\rho_{max} = 0.38$ e Å^{-3}
4 restraints	$\Delta\rho_{min} = -0.27$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.5000	0.30069 (5)	0.7500	0.01561 (13)
N1	0.58142 (7)	0.3092 (2)	0.73473 (13)	0.0179 (3)
O1	0.90563 (6)	0.2232 (2)	0.96391 (12)	0.0266 (3)
O2	0.96160 (6)	0.29413 (19)	0.87580 (12)	0.0242 (3)
O1W	0.46891 (6)	0.0848 (2)	0.64084 (11)	0.0199 (3)
O2W	0.53247 (6)	0.5047 (2)	0.86819 (11)	0.0208 (3)
C1	0.91223 (9)	0.2740 (3)	0.88189 (16)	0.0197 (4)
C2	0.85662 (8)	0.3156 (3)	0.78537 (16)	0.0172 (4)
C3	0.85969 (8)	0.3652 (3)	0.69003 (17)	0.0208 (4)
H3	0.8970	0.3732	0.6845	0.025*
C4	0.80768 (8)	0.4029 (3)	0.60302 (16)	0.0220 (4)
H4	0.8096	0.4366	0.5377	0.026*
C5	0.75295 (8)	0.3919 (3)	0.61016 (15)	0.0205 (4)
H5	0.7178	0.4188	0.5500	0.025*
C6	0.74932 (8)	0.3414 (3)	0.70535 (15)	0.0176 (4)
C7	0.80178 (8)	0.3043 (3)	0.79252 (16)	0.0173 (4)
H7	0.8000	0.2706	0.8580	0.021*
C8	0.69121 (8)	0.3288 (3)	0.71474 (16)	0.0173 (4)
C9	0.68658 (8)	0.3575 (3)	0.81138 (16)	0.0198 (4)
H9	0.7210	0.3856	0.8727	0.024*
C10	0.63215 (9)	0.3452 (3)	0.81801 (16)	0.0205 (4)
H10	0.6305	0.3632	0.8851	0.025*

C11	0.58576 (9)	0.2824 (3)	0.64134 (16)	0.0199 (4)
H11A	0.5505	0.2566	0.5811	0.024*
C12	0.63867 (8)	0.2903 (3)	0.62852 (16)	0.0198 (4)
H12A	0.6392	0.2694	0.5608	0.024*
H11	0.4524 (11)	0.124 (4)	0.5786 (11)	0.048 (9)*
H12	0.4935 (8)	0.004 (3)	0.6396 (17)	0.023 (6)*
H21	0.5473 (10)	0.452 (3)	0.9275 (11)	0.030 (7)*
H22	0.5096 (10)	0.591 (3)	0.869 (2)	0.043 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01032 (18)	0.0186 (2)	0.0183 (2)	0.000	0.00608 (14)	0.000
N1	0.0125 (7)	0.0184 (8)	0.0222 (9)	−0.0001 (6)	0.0061 (7)	0.0022 (7)
O1	0.0189 (7)	0.0361 (9)	0.0215 (8)	−0.0012 (6)	0.0043 (6)	0.0023 (6)
O2	0.0118 (7)	0.0227 (8)	0.0362 (9)	0.0008 (5)	0.0077 (6)	0.0012 (6)
O1W	0.0155 (7)	0.0222 (8)	0.0216 (8)	0.0010 (6)	0.0071 (6)	−0.0019 (6)
O2W	0.0156 (7)	0.0225 (8)	0.0226 (8)	0.0028 (6)	0.0056 (6)	−0.0022 (6)
C1	0.0154 (9)	0.0154 (9)	0.0259 (11)	−0.0002 (7)	0.0056 (8)	−0.0042 (8)
C2	0.0149 (9)	0.0145 (9)	0.0214 (10)	−0.0026 (7)	0.0064 (8)	−0.0045 (8)
C3	0.0149 (9)	0.0215 (10)	0.0294 (11)	−0.0027 (8)	0.0122 (8)	−0.0026 (8)
C4	0.0212 (10)	0.0277 (11)	0.0202 (10)	−0.0032 (8)	0.0115 (8)	−0.0003 (9)
C5	0.0158 (9)	0.0234 (10)	0.0206 (10)	−0.0007 (8)	0.0054 (8)	−0.0002 (8)
C6	0.0135 (9)	0.0176 (9)	0.0223 (10)	−0.0020 (7)	0.0078 (8)	−0.0033 (7)
C7	0.0156 (9)	0.0179 (9)	0.0187 (9)	0.0002 (7)	0.0071 (8)	0.0002 (8)
C8	0.0149 (9)	0.0163 (9)	0.0205 (10)	0.0014 (7)	0.0069 (8)	0.0024 (7)
C9	0.0130 (9)	0.0242 (10)	0.0204 (10)	0.0011 (8)	0.0047 (8)	0.0004 (8)
C10	0.0175 (9)	0.0255 (10)	0.0198 (10)	0.0014 (8)	0.0090 (8)	0.0003 (8)
C11	0.0139 (9)	0.0237 (10)	0.0210 (10)	−0.0004 (8)	0.0057 (8)	0.0008 (8)
C12	0.0167 (10)	0.0230 (10)	0.0196 (10)	−0.0007 (8)	0.0071 (8)	−0.0007 (8)

Geometric parameters (Å, °)

Ni1—O1W	2.0627 (14)	C3—C4	1.388 (3)
Ni1—O1W^{i}	2.0627 (14)	C3—H3	0.9500
Ni1—O2W	2.0811 (14)	C4—C5	1.389 (3)
Ni1—O2W^{i}	2.0811 (14)	C4—H4	0.9500
Ni1—N1^{i}	2.0931 (16)	C5—C6	1.396 (3)
Ni1—N1	2.0931 (16)	C5—H5	0.9500
N1—C10	1.342 (3)	C6—C7	1.395 (3)
N1—C11	1.346 (2)	C6—C8	1.486 (3)
O1—C1	1.256 (3)	C7—H7	0.9500
O2—C1	1.256 (2)	C8—C12	1.392 (3)
O1W—H11	0.838 (10)	C8—C9	1.396 (3)
O1W—H12	0.834 (10)	C9—C10	1.378 (3)
O2W—H21	0.840 (10)	C9—H9	0.9500
O2W—H22	0.833 (10)	C10—H10	0.9500
C1—C2	1.511 (3)	C11—C12	1.380 (3)

C2—C3	1.390 (3)	C11—H11A	0.9500
C2—C7	1.391 (3)	C12—H12A	0.9500
O1W—Ni1—O1W^{i}	84.85 (8)	C4—C3—C2	119.26 (17)
O1W—Ni1—O2W	176.09 (6)	C4—C3—H3	120.4
O1W^{i}—Ni1—O2W	91.32 (6)	C2—C3—H3	120.4
O1W—Ni1—O2W^{i}	91.32 (6)	C3—C4—C5	120.92 (18)
O1W^{i}—Ni1—O2W^{i}	176.09 (6)	C3—C4—H4	119.5
O2W—Ni1—O2W^{i}	92.51 (8)	C5—C4—H4	119.5
O1W—Ni1—N1^{i}	90.11 (6)	C4—C5—C6	120.31 (18)
O1W^{i}—Ni1—N1^{i}	92.32 (6)	C4—C5—H5	119.8
O2W—Ni1—N1^{i}	89.24 (6)	C6—C5—H5	119.8
O2W^{i}—Ni1—N1^{i}	88.48 (6)	C7—C6—C5	118.45 (17)
O1W—Ni1—N1	92.32 (6)	C7—C6—C8	120.35 (17)
O1W^{i}—Ni1—N1	90.11 (6)	C5—C6—C8	121.19 (17)
O2W—Ni1—N1	88.48 (6)	C2—C7—C6	121.21 (18)
O2W^{i}—Ni1—N1	89.24 (6)	C2—C7—H7	119.4
N1^{i}—Ni1—N1	176.71 (9)	C6—C7—H7	119.4
C10—N1—C11	116.48 (16)	C12—C8—C9	116.40 (17)
C10—N1—Ni1	121.33 (13)	C12—C8—C6	122.37 (18)
C11—N1—Ni1	122.18 (13)	C9—C8—C6	121.23 (17)
Ni1—O1W—H11	113 (2)	C10—C9—C8	120.12 (18)
Ni1—O1W—H12	117.0 (16)	C10—C9—H9	119.9
H11—O1W—H12	105 (2)	C8—C9—H9	119.9
Ni1—O2W—H21	109.7 (18)	N1—C10—C9	123.49 (18)
Ni1—O2W—H22	117.8 (19)	N1—C10—H10	118.3
H21—O2W—H22	110 (2)	C9—C10—H10	118.3
O1—C1—O2	124.36 (19)	N1—C11—C12	123.49 (19)
O1—C1—C2	116.99 (17)	N1—C11—H11A	118.3
O2—C1—C2	118.65 (18)	C12—C11—H11A	118.3
C3—C2—C7	119.85 (18)	C11—C12—C8	120.03 (19)
C3—C2—C1	120.82 (17)	C11—C12—H12A	120.0
C7—C2—C1	119.32 (18)	C8—C12—H12A	120.0
O1W—Ni1—N1—C10	−144.22 (15)	C3—C2—C7—C6	0.1 (3)
O1W^{i}—Ni1—N1—C10	−59.36 (15)	C1—C2—C7—C6	−179.93 (17)
O2W—Ni1—N1—C10	31.96 (15)	C5—C6—C7—C2	−0.4 (3)
O2W^{i}—Ni1—N1—C10	124.49 (15)	C8—C6—C7—C2	−179.88 (17)
O1W—Ni1—N1—C11	36.93 (15)	C7—C6—C8—C12	−154.18 (19)
O1W^{i}—Ni1—N1—C11	121.79 (15)	C5—C6—C8—C12	26.4 (3)
O2W—Ni1—N1—C11	−146.89 (15)	C7—C6—C8—C9	26.6 (3)
O2W^{i}—Ni1—N1—C11	−54.36 (15)	C5—C6—C8—C9	−152.89 (19)
O1—C1—C2—C3	−177.38 (18)	C12—C8—C9—C10	0.6 (3)
O2—C1—C2—C3	3.5 (3)	C6—C8—C9—C10	179.95 (18)
O1—C1—C2—C7	2.7 (3)	C11—N1—C10—C9	0.8 (3)
O2—C1—C2—C7	−176.42 (17)	Ni1—N1—C10—C9	−178.14 (15)
C7—C2—C3—C4	0.0 (3)	C8—C9—C10—N1	−1.1 (3)

C1—C2—C3—C4	−179.89 (18)	C10—N1—C11—C12	0.0 (3)
C2—C3—C4—C5	0.1 (3)	Ni1—N1—C11—C12	178.89 (14)
C3—C4—C5—C6	−0.4 (3)	N1—C11—C12—C8	−0.4 (3)
C4—C5—C6—C7	0.5 (3)	C9—C8—C12—C11	0.1 (3)
C4—C5—C6—C8	179.99 (18)	C6—C8—C12—C11	−179.22 (18)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H11···O1^{ii}	0.84 (1)	1.88 (1)	2.682 (2)	160 (3)
O1w—H12···O2^{iii}	0.83 (1)	1.91 (1)	2.734 (2)	170 (2)
O2w—H21···O1^{iv}	0.84 (1)	1.93 (1)	2.732 (2)	159 (2)
O2w—H22···O2^{v}	0.83 (1)	1.88 (1)	2.711 (2)	177 (3)

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

Fig. 1