Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis[5-(pyrazin-2-yl)-5*H*-tetrazolato-κN^1]nickel(II)

Sheng-Di Fan and Ju-Tao Liu*

School of Life Science, Dalian Nationalities University, Dalian 116600, People's Republic of China
Correspondence e-mail: jutaoliu@yahoo.com.cn

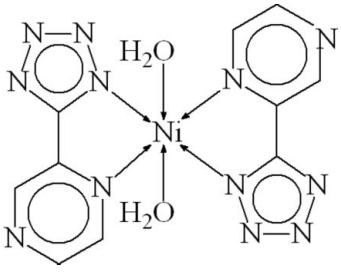
Received 17 June 2007; accepted 26 June 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.024; wR factor = 0.064; data-to-parameter ratio = 11.8.

In the title compound, $[Ni(C_5H_3N_6)_2(H_2O)_2]$, the central Ni atom is located on a centre of inversion and is coordinated by two chelating pyrazinyltetrazolate ligands and two water molecules in a slightly distorted octahedral geometry [Ni—N = 2.082 (2) and 2.125 (2) Å, and Ni—O = 2.068 (2) Å]. These molecules are linked by O—H···N hydrogen bonds into a three-dimensional network.

Related literature

For related literature, see: Deng *et al.* (2007); Liu *et al.* (2007*a*, 2007*b*); Luo *et al.* (2006); Song & Xi (2006); Zeng *et al.* (2007).



Experimental

Crystal data

$[Ni(C_5H_3N_6)_2(H_2O)_2]$
M_r = 389.01
Monoclinic, $P2_1/n$
a = 6.1539 (11) Å
b = 11.3456 (19) Å
c = 10.6126 (18) Å
β = 105.845 (2)°
V = 712.8 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.40 mm^{-1}
T = 294 (2) K
0.22 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.948, T_{max} = 1.000
3871 measured reflections
1451 independent reflections
1223 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.065
S = 1.06
1451 reflections
123 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—N1	2.1245 (16)	Ni1—O1	2.0679 (15)
Ni1—N6	2.0823 (15)		
O1^{i}—Ni1—N6	92.57 (7)	O1—Ni1—N1	89.38 (6)
O1—Ni1—N6	87.43 (7)	N6—Ni1—N1	79.68 (6)
O1^{i}—Ni1—N1	90.62 (6)	N6^{i}—Ni1—N1	100.32 (6)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N5^{ii}	0.843 (10)	2.037 (12)	2.863 (2)	166 (2)
O1—H1B···N3^{iii}	0.850 (10)	1.913 (11)	2.761 (2)	175 (3)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97*; molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

The authors thank Dalian Nationalities University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2242).

References

Bruker (1998). *SMART* (Version 5.051), *SAINT* (Version 5.01), *SADABS* (Version 2.03) and *SHELXTL* (Version 6.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Deng, H., Qiu, Y.-C., Zeng, R.-H. & Sun, F. (2007). *Acta Cryst.* E**63**, m450–m451.
Liu, J.-T., Fan, S.-D. & Ng, S. W. (2007*a*). *Acta Cryst.* E**63**, m1651.
Liu, J.-T., Fan, S.-D. & Ng, S. W. (2007*b*). *Acta Cryst.* E**63**, m1652.
Luo, J., Zhang, X.-R., Cui, L.-L., Dai, W.-Q. & Liu, B.-S. (2006). *Acta Cryst.* C**62**, m614–m616.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Song, W.-D. & Xi, D.-L. (2006). *Acta Cryst.* E**62**, m2841–m2842.
Zeng, R.-H., Cui, Y.-C., Liu, Z.-H., Li, Y.-H. & Deng, H. (2007). *Acta Cryst.* E**63**, m1591.

  doi:10.1107/S160053680703111X

supplementary materials

Acta Cryst. (2007). E**63**, m2034 [**doi:10.1107/S160053680703111X**]

Diaquabis[5-(pyrazin-2-yl)-5*H*-tetrazolato-κN^1]nickel(II)

S.-D. Fan and J.-T. Liu

Comment

Recently, we (Liu *et al.*, 2007*a*, 2007*b*) and others (Deng *et al.*, 2007; Luo *et al.*, 2006; Song *et al.*, 2006; Zeng *et al.*, 2007) reported the crystal structures of Cu(II), Pb(II), Mn(II), Zn(II), Co(II) and Fe(II) complexes with the 5-(2-pyrazinyl)-5*H*-tetrazolate ligand. Except for that of the Pb(II) (one dimensional), these complexes adopt a mononuclear structure, being isomorphous with the title compound, $C_{10}H_{10}NiN_{12}O_2$ (I) (Fig. 1). The central Ni atom, located on a center of inversion, is coordinated by two water molecules and two ligand molecules to form a slightly distorted octahedral geometry. Furthermore, a three-dimensional supramolecular framework (Fig. 2) is formed by the intermolecular O—H—N hydrogen-bond interactions. The hydrogen bond parameters are listed in Table 2.

Experimental

A 5 ml of $NiCl_2{\cdot}6H_2O$ (48 mg, 0.2 mmol) solution in methanol was layered on a 10 ml of 2-(1*H*-tetrazol-5-yl)pyrazine (60 mg, 0.4 mmol) solution in methanol/water (1:1), and allowed to stand. After two months, purple crystals of (I) were isolated in about 20% yield.

Refinement

H atoms bound to carbon were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C,*N*). The H atoms of the water molecules were located in Fourier difference maps and refined with isotropic displacement parameters set at 1.5 times those of the parent O atoms.

Figures

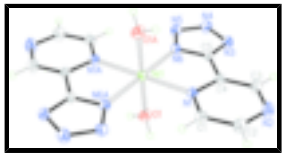


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. [symmetry code: (A) −*x*, 2 − *y*, 2 − *z*.]

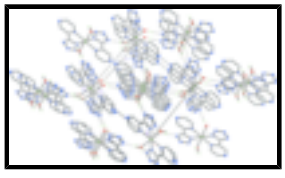


Fig. 2. Three-dimensional hydrogen-bonded network.

Diaquabis[5-(pyrazin-2-yl)-5H-tetrazolato-κN^1]nickel(II)

Crystal data

$[Ni(C_5H_3N_6)_2(H_2O)_2]$	F_{000} = 396
M_r = 389.01	D_x = 1.812 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2310 reflections
a = 6.1539 (11) Å	θ = 2.7–26.3º
b = 11.3456 (19) Å	μ = 1.40 mm^{-1}
c = 10.6126 (18) Å	T = 294 (2) K
β = 105.845 (2)º	Block, purple
V = 712.8 (2) Å^3	0.22 × 0.20 × 0.20 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	1451 independent reflections
Radiation source: fine-focus sealed tube	1223 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.024
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 2.7º
Absorption correction: multi-scan (SADABS; Bruker, 1998)	h = −6→7
T_{min} = 0.948, T_{max} = 1.000	k = −11→14
3871 measured reflections	l = −13→11

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.024	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.065	$w = 1/[\sigma^2(F_o^2) + (0.0305P)^2 + 0.3065P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$
1451 reflections	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
123 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.0000	1.0000	1.0000	0.02261 (12)
N1	0.1308 (3)	1.17316 (13)	0.99873 (14)	0.0247 (3)
N2	0.2383 (3)	1.41026 (16)	0.9762 (2)	0.0456 (5)
N3	−0.4243 (3)	1.25269 (15)	0.79180 (16)	0.0328 (4)
N4	−0.5848 (3)	1.16844 (16)	0.76264 (17)	0.0367 (4)
N5	−0.5029 (3)	1.06965 (15)	0.82244 (16)	0.0333 (4)
N6	−0.2877 (3)	1.08776 (14)	0.89169 (15)	0.0275 (4)
C1	0.3369 (3)	1.21598 (18)	1.05560 (19)	0.0313 (4)
H1C	0.4478	1.1655	1.1038	0.038*
C2	0.3893 (4)	1.3336 (2)	1.0445 (2)	0.0391 (5)
H2A	0.5343	1.3600	1.0859	0.047*
C3	0.0328 (4)	1.36789 (18)	0.9198 (2)	0.0385 (5)
H3A	−0.0775	1.4188	0.8718	0.046*
C4	−0.0221 (3)	1.25059 (17)	0.93032 (17)	0.0260 (4)
C5	−0.2457 (3)	1.20037 (16)	0.87052 (18)	0.0255 (4)
O1	0.0740 (3)	0.96615 (14)	0.82476 (15)	0.0369 (4)
H1A	0.204 (2)	0.985 (2)	0.819 (3)	0.055 (8)*
H1B	0.037 (5)	0.8993 (14)	0.789 (3)	0.070 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.02113 (18)	0.01848 (18)	0.02574 (18)	−0.00025 (13)	0.00220 (13)	0.00169 (13)
N1	0.0232 (8)	0.0255 (8)	0.0244 (8)	−0.0001 (6)	0.0047 (6)	−0.0001 (6)
N2	0.0394 (11)	0.0286 (10)	0.0617 (12)	−0.0085 (8)	0.0018 (9)	0.0004 (9)
N3	0.0283 (9)	0.0323 (9)	0.0348 (9)	0.0015 (7)	0.0037 (7)	0.0064 (7)
N4	0.0278 (9)	0.0391 (10)	0.0382 (9)	−0.0006 (8)	0.0006 (7)	0.0055 (8)
N5	0.0250 (9)	0.0338 (10)	0.0376 (9)	−0.0039 (7)	0.0027 (7)	0.0004 (8)
N6	0.0215 (8)	0.0261 (8)	0.0321 (8)	−0.0012 (7)	0.0025 (7)	0.0012 (7)
C1	0.0252 (10)	0.0340 (11)	0.0311 (10)	0.0006 (8)	0.0014 (8)	0.0000 (8)
C2	0.0312 (11)	0.0387 (12)	0.0427 (12)	−0.0085 (9)	0.0019 (9)	−0.0061 (10)
C3	0.0361 (12)	0.0263 (11)	0.0485 (13)	−0.0002 (9)	0.0038 (10)	0.0043 (9)

C4	0.0258 (10)	0.0252 (9)	0.0263 (9)	0.0008 (8)	0.0056 (7)	0.0012 (8)
C5	0.0248 (9)	0.0238 (9)	0.0276 (9)	0.0021 (8)	0.0065 (8)	0.0022 (7)
O1	0.0389 (9)	0.0367 (9)	0.0376 (8)	−0.0126 (7)	0.0150 (7)	−0.0101 (7)

Geometric parameters (Å, °)

Ni1—N1	2.1245 (16)	N4—N5	1.319 (2)
Ni1—N6	2.0823 (15)	N5—N6	1.343 (2)
Ni1—O1	2.0679 (15)	N6—C5	1.335 (2)
Ni1—O1^{i}	2.0679 (15)	C1—C2	1.386 (3)
Ni1—N6^{i}	2.0823 (16)	C1—H1C	0.9300
Ni1—N1^{i}	2.1245 (16)	C2—H2A	0.9300
N1—C1	1.338 (2)	C3—C4	1.385 (3)
N1—C4	1.346 (2)	C3—H3A	0.9300
N2—C3	1.332 (3)	C4—C5	1.464 (3)
N2—C2	1.333 (3)	O1—H1A	0.843 (10)
N3—C5	1.325 (2)	O1—H1B	0.850 (10)
N3—N4	1.348 (2)		
O1^{i}—Ni1—O1	180.000 (1)	C5—N6—N5	105.16 (15)
O1^{i}—Ni1—N6	92.57 (7)	C5—N6—Ni1	112.10 (12)
O1—Ni1—N6	87.43 (7)	N5—N6—Ni1	142.32 (13)
O1^{i}—Ni1—N6^{i}	87.43 (7)	N1—C1—C2	121.68 (19)
O1—Ni1—N6^{i}	92.57 (7)	N1—C1—H1C	119.2
N6—Ni1—N6^{i}	180.000 (1)	C2—C1—H1C	119.2
O1^{i}—Ni1—N1	90.62 (6)	N2—C2—C1	122.0 (2)
O1—Ni1—N1	89.38 (6)	N2—C2—H2A	119.0
N6—Ni1—N1	79.68 (6)	C1—C2—H2A	119.0
N6^{i}—Ni1—N1	100.32 (6)	N2—C3—C4	122.2 (2)
O1^{i}—Ni1—N1^{i}	89.38 (6)	N2—C3—H3A	118.9
O1—Ni1—N1^{i}	90.62 (6)	C4—C3—H3A	118.9
N6—Ni1—N1^{i}	100.32 (6)	N1—C4—C3	121.38 (18)
N6^{i}—Ni1—N1^{i}	79.68 (6)	N1—C4—C5	114.57 (17)
N1—Ni1—N1^{i}	180.0	C3—C4—C5	124.06 (18)
C1—N1—C4	116.31 (17)	N3—C5—N6	111.69 (17)
C1—N1—Ni1	130.31 (13)	N3—C5—C4	128.19 (18)
C4—N1—Ni1	113.38 (12)	N6—C5—C4	120.11 (16)
C3—N2—C2	116.37 (19)	Ni1—O1—H1A	117.2 (19)
C5—N3—N4	104.87 (16)	Ni1—O1—H1B	118 (2)
N5—N4—N3	109.39 (16)	H1A—O1—H1B	110 (3)
N4—N5—N6	108.90 (16)		
O1^{i}—Ni1—N1—C1	85.06 (17)	Ni1—N1—C1—C2	−179.17 (15)
O1—Ni1—N1—C1	−94.94 (17)	C3—N2—C2—C1	0.6 (3)
N6—Ni1—N1—C1	177.56 (18)	N1—C1—C2—N2	−0.4 (3)
N6^{i}—Ni1—N1—C1	−2.44 (18)	C2—N2—C3—C4	−0.4 (3)
O1^{i}—Ni1—N1—C4	−94.15 (13)	C1—N1—C4—C3	0.1 (3)

O1—Ni1—N1—C4	85.85 (13)	Ni1—N1—C4—C3	179.45 (16)
N6—Ni1—N1—C4	−1.65 (13)	C1—N1—C4—C5	−179.58 (17)
N6^{i}—Ni1—N1—C4	178.35 (13)	Ni1—N1—C4—C5	−0.2 (2)
C5—N3—N4—N5	0.0 (2)	N2—C3—C4—N1	0.1 (3)
N3—N4—N5—N6	0.1 (2)	N2—C3—C4—C5	179.8 (2)
N4—N5—N6—C5	−0.1 (2)	N4—N3—C5—N6	0.0 (2)
N4—N5—N6—Ni1	−171.40 (16)	N4—N3—C5—C4	178.99 (18)
O1^{i}—Ni1—N6—C5	93.53 (14)	N5—N6—C5—N3	0.1 (2)
O1—Ni1—N6—C5	−86.47 (14)	Ni1—N6—C5—N3	174.35 (13)
N1—Ni1—N6—C5	3.37 (13)	N5—N6—C5—C4	−179.04 (16)
N1^{i}—Ni1—N6—C5	−176.63 (13)	Ni1—N6—C5—C4	−4.8 (2)
O1^{i}—Ni1—N6—N5	−95.5 (2)	N1—C4—C5—N3	−175.51 (19)
O1—Ni1—N6—N5	84.5 (2)	C3—C4—C5—N3	4.8 (3)
N1—Ni1—N6—N5	174.3 (2)	N1—C4—C5—N6	3.4 (3)
N1^{i}—Ni1—N6—N5	−5.7 (2)	C3—C4—C5—N6	−176.24 (19)
C4—N1—C1—C2	0.0 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···N5^{ii}	0.843 (10)	2.037 (12)	2.863 (2)	166 (2)
O1—H1B···N3^{iii}	0.850 (10)	1.913 (11)	2.761 (2)	175 (3)

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

Fig. 1

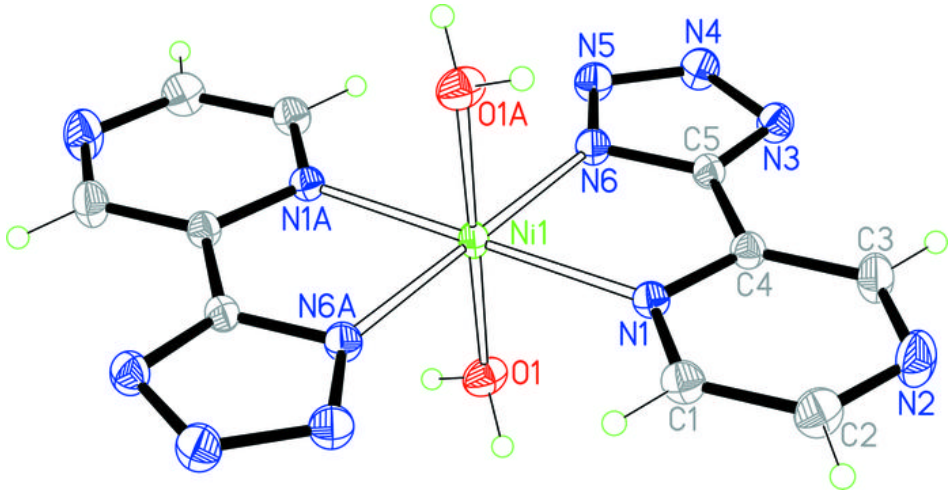


Fig. 2