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catena-Poly[[tetraaqua[*trans*-1,2-bis(4-pyridyl)ethene-κ^2N:N']nickel(II)] dinitrate]

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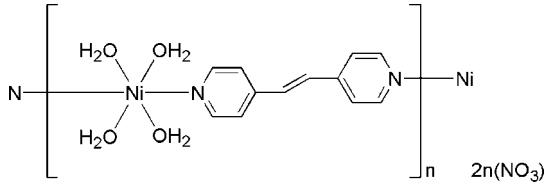
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.009 Å; R factor = 0.068; wR factor = 0.238; data-to-parameter ratio = 13.2.

In the title compound, $\{[Ni(C_{12}H_{10}N_2)(H_2O)_4](NO_3)_2\}_n$, the Ni^{II} ion, lying on a crystallographic inversion center, has a distorted octahedral coordination sphere comprising four water ligands and two N-atom donors from the *trans*-related 1,2-bis(4-pyridyl)ethene ligands, which also have crystallographic inversion symmetry. These ligands bridge the Ni^{II} complex units, forming chains extending along the [110] and [$\bar{1}$10] directions. The nitrate counter-anions stabilize the crystal structure through water–nitrate O—H···O hydrogen bonds.

Related literature

For interactions of metal ions with amino acids, see: Daniele *et al.* (2008); Parkin (2004); Tshuva & Lippard (2004). For related complexes,see: Lee *et al.* (2008); Yu *et al.* (2008); Park *et al.* (2008); Shin *et al.* (2009); Yu *et al.* (2009, 2010); Kim *et al.* (2011).



Experimental

Crystal data

$[Ni(C_{12}H_{10}N_2)(H_2O)_4](NO_3)_2$
M_r = 436.99
Monoclinic, $P2_1/n$
a = 7.415 (3) Å
b = 11.426 (4) Å
c = 10.950 (4) Å
β = 97.307 (7)°
V = 920.1 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.11 mm^{-1}
T = 293 K
0.15 × 0.08 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
4954 measured reflections
1799 independent reflections
1116 reflections with $I > 2\sigma(I)$
R_{int} = 0.173

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.238
S = 1.14
1799 reflections
136 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.08 e Å^{-3}
$\Delta\rho_{min}$ = −1.86 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2B···O3^{i}	0.93 (7)	2.28 (8)	3.176 (9)	162 (8)
O2—H2A···O5^{ii}	0.93 (6)	2.14 (7)	3.068 (8)	176 (7)
O1—H1B···O3^{iii}	0.93 (4)	2.29 (2)	3.212 (9)	170 (8)
O1—H1A···O4^{iv}	0.93 (6)	2.37 (3)	3.252 (8)	158 (7)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: ZS2096).

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supporting information

Acta Cryst. (2011). E**67**, m390 [doi:10.1107/S1600536811007021]

catena-Poly[[tetraaqua[*trans*-1,2-bis(4-pyridyl)ethene-κ^2N:N']nickel(II)] dinitrate]

Min Young Hyun, Pan-Gi Kim, Cheal Kim and Youngmee Kim

S1. Comment

The interaction of transition metal ions with biologically active molecules such as amino acids and various acids is very important in biological systems (Daniele *et al.*, 2008; Parkin, 2004; Tshuva & Lippard, 2004). In attempting to model the interaction, we have extensively studied the interaction of the transition metal carboxylates e.g. copper(II), cadmium(II), and zinc(II) benzoates with a variety of spacers such as quinoxaline, 6-methylquinoline, 3-methylquinoline, *trans*-1-(2-pyridyl)-2-(4-pyridyl)ethylene, and di-2-pyridyl ketone (Lee *et al.*, 2008; Yu *et al.*, 2008; Park *et al.*, 2008; Shin *et al.*, 2009; Yu *et al.*, 2009; Yu *et al.*, 2010; Kim *et al.*, 2011). However, nickel as a metal ion source has rarely been used. In this work, we have employed nickel(II) trimethylacetate as a building block and *trans*-1,2-bis(4-pyridyl)ethene as a ligand. We report here on the structure of a new complex poly[tetraqua[*trans*-1,2-bis(4-pyridyl)ethene]nickel(II) dinitrate].

In the crystal structure of the title compound, $[Ni(C_{12}H_{10}N_2)(H_2O)_4] \cdot 2(NO_3)]_n$, the Ni^{II} ion lies on a crystallographic inversion center with the distorted octahedral coordination sphere comprising four water ligands and two N donors from the *trans*-related 1,2-bis(4-pyridyl)ethene ligands, which also have crystallographic inversion symmetry (Fig. 1). These ligands bridge the Ni^{II} complex units to form a one-dimensional chain structure. The nitrate counter-anions stabilize the crystal structure through water O—H···$O_{nitrate}$ hydrogen bonds (Table 1).

S2. Experimental

36.4 mg (0.125 mmol) of $Ni(NO_3)_2{\cdot}6H_2O$ and 29.0 mg (0.25 mmol) of $(CH_3)_3CCOOH$ and 29.5 mg (0. 25 mmol) of NH_4OH were dissolved in 4 ml of methanol and carefully layered with 4 ml of a chloroform solution of *trans*-1,2-bis(4-pyridyl)ethene (47.0 mg, 0.25 mmol). Crystals of the title compound suitable for X-ray analysis were obtained within a month.

S3. Refinement

H atoms were placed in calculated positions with C—H distances of 0.93 Å (pyridyl) and included in the refinement with a riding-motion approximation with $U_{iso}(H) = 1.2U_{eq}(C)$. The water H atoms were located in a difference Fourier, and refined isotropically with O—H restraints (0.93 Å).

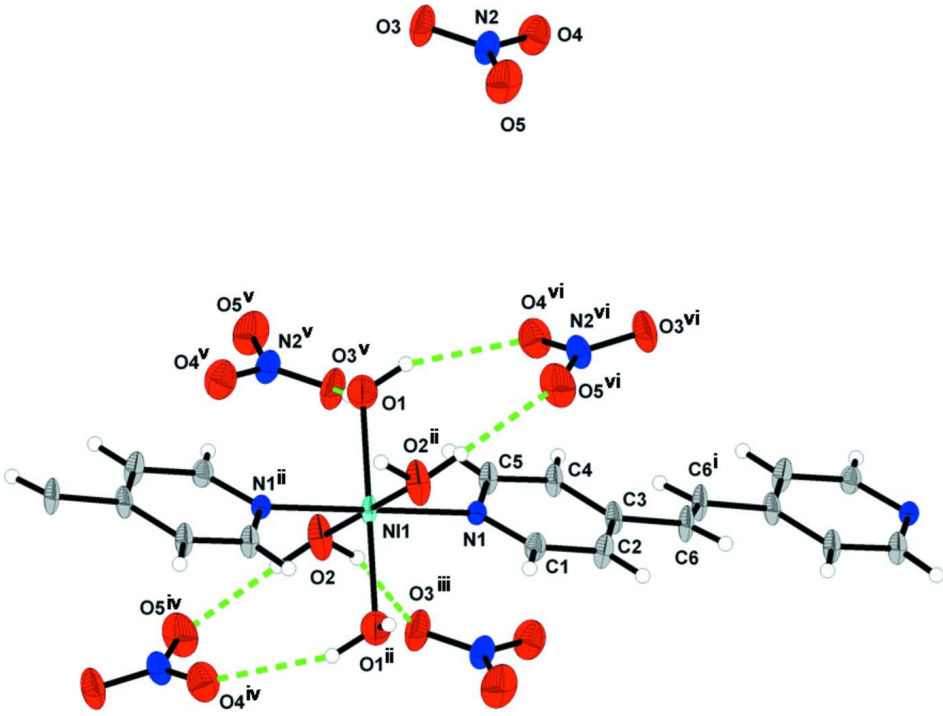

Figure 1

A fragment of one-dimensional chain structure of the title compound showing the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Inter-species hydrogen bonds are shown as dashed lines. For symmetry codes: (i) (-*x* + 1, -*y* + 1, -*z*); (ii) -*x*, -*y* + 2, -*z*). For other codes, see Table 1.

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Crystal data

$[Ni(C_{12}H_{10}N_2)(H_2O)_4](NO_3)_2$
M_r = 436.99
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 7.415 (3) Å
b = 11.426 (4) Å
c = 10.950 (4) Å
β = 97.307 (7)°
V = 920.1 (6) Å^3
Z = 2
$F(000)$ = 452
D_x = 1.577 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1268 reflections
θ = 2.6–23.4°
μ = 1.11 mm^{-1}
T = 293 K
Block, brown
0.15 × 0.08 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
4954 measured reflections
1799 independent reflections
1116 reflections with $I > 2\sigma(I)$
R_{int} = 0.173
θ_{max} = 26.0°, θ_{min} = 2.6°
h = −8→9
k = −11→14
l = −11→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.238$
$S = 1.14$
1799 reflections
136 parameters
4 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
$w = 1/[\sigma^2(F_o^2) + (0.1257P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.08$ e Å^{-3}
$\Delta\rho_{min} = -1.86$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.0496 (8)	0.7389 (5)	−0.0578 (7)	0.0346 (15)
H1	−0.0705	0.7450	−0.0939	0.042*
C2	0.1365 (8)	0.6328 (5)	−0.0637 (7)	0.0414 (18)
H2	0.0758	0.5697	−0.1038	0.050*
C3	0.3181 (8)	0.6207 (5)	−0.0086 (7)	0.0364 (16)
C4	0.3954 (8)	0.7169 (5)	0.0524 (7)	0.0374 (16)
H4	0.5137	0.7129	0.0923	0.045*
C5	0.2991 (7)	0.8183 (5)	0.0544 (7)	0.0350 (16)
H5	0.3542	0.8814	0.0981	0.042*
C6	0.4117 (9)	0.5087 (5)	−0.0174 (8)	0.0431 (19)
H6	0.3429	0.4452	−0.0495	0.052*
N1	0.1284 (6)	0.8326 (4)	−0.0032 (5)	0.0271 (11)
Ni1	0.0000	1.0000	0.0000	0.0287 (4)
O1	0.0809 (9)	1.0135 (4)	0.1951 (7)	0.0630 (17)
H1A	0.098 (12)	0.946 (4)	0.242 (7)	0.076*
H1B	0.200 (4)	1.036 (7)	0.189 (9)	0.076*
O2	0.2381 (6)	1.0811 (4)	−0.0466 (7)	0.0666 (18)
H2A	0.226 (11)	1.148 (5)	−0.095 (7)	0.080*
H2B	0.306 (10)	1.024 (6)	−0.080 (9)	0.080*
N2	0.4686 (7)	0.8286 (5)	0.7660 (6)	0.0481 (16)
O3	0.4935 (7)	0.9318 (4)	0.8009 (6)	0.0684 (17)
O4	0.5938 (8)	0.7571 (5)	0.7875 (7)	0.0699 (18)
O5	0.3209 (7)	0.7990 (5)	0.7106 (7)	0.083 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.031 (3)	0.026 (3)	0.046 (4)	0.005 (2)	0.000 (3)	−0.002 (3)
C2	0.030 (3)	0.023 (3)	0.069 (5)	0.003 (2)	−0.005 (3)	−0.010 (3)
C3	0.030 (3)	0.018 (3)	0.060 (5)	0.009 (2)	−0.001 (3)	0.004 (3)
C4	0.028 (3)	0.018 (3)	0.064 (5)	0.004 (2)	−0.005 (3)	0.000 (3)
C5	0.024 (3)	0.020 (3)	0.060 (5)	0.001 (2)	0.001 (3)	−0.001 (3)
C6	0.037 (3)	0.014 (3)	0.076 (6)	0.009 (2)	0.000 (3)	−0.003 (3)
N1	0.027 (2)	0.022 (2)	0.033 (3)	0.0061 (19)	0.005 (2)	−0.001 (2)
Ni1	0.0214 (6)	0.0136 (6)	0.0485 (8)	0.0038 (4)	−0.0049 (5)	−0.0014 (4)
O1	0.066 (4)	0.051 (3)	0.066 (4)	0.000 (3)	−0.013 (3)	0.000 (3)
O2	0.044 (3)	0.035 (3)	0.121 (6)	0.003 (2)	0.010 (3)	0.012 (3)
N2	0.040 (3)	0.036 (3)	0.064 (5)	−0.003 (2)	−0.012 (3)	−0.010 (3)
O3	0.064 (3)	0.035 (3)	0.098 (5)	−0.008 (2)	−0.018 (3)	−0.016 (3)
O4	0.059 (3)	0.059 (3)	0.091 (5)	0.017 (3)	0.006 (3)	−0.008 (3)
O5	0.055 (3)	0.074 (4)	0.110 (6)	−0.017 (3)	−0.030 (4)	−0.016 (4)

Geometric parameters (Å, º)

C1—N1	1.326 (7)	N1—Ni1	2.138 (4)
C1—C2	1.378 (8)	Ni1—O2	2.113 (5)
C1—H1	0.9300	Ni1—O2^{ii}	2.113 (5)
C2—C3	1.411 (8)	Ni1—N1^{ii}	2.138 (4)
C2—H2	0.9300	Ni1—O1^{ii}	2.149 (7)
C3—C4	1.373 (8)	Ni1—O1	2.149 (7)
C3—C6	1.465 (8)	O1—H1A	0.93 (6)
C4—C5	1.362 (7)	O1—H1B	0.93 (4)
C4—H4	0.9300	O2—H2A	0.93 (6)
C5—N1	1.350 (7)	O2—H2B	0.93 (7)
C5—H5	0.9300	N2—O5	1.231 (6)
C6—C6^{i}	1.331 (13)	N2—O4	1.236 (7)
C6—H6	0.9300	N2—O3	1.245 (7)
N1—C1—C2	123.4 (5)	O2^{ii}—Ni1—N1^{ii}	90.05 (18)
N1—C1—H1	118.3	O2—Ni1—N1	90.05 (18)
C2—C1—H1	118.3	O2^{ii}—Ni1—N1	89.95 (18)
C1—C2—C3	119.5 (5)	N1^{ii}—Ni1—N1	180.0
C1—C2—H2	120.3	O2—Ni1—O1^{ii}	85.9 (3)
C3—C2—H2	120.3	O2^{ii}—Ni1—O1^{ii}	94.1 (3)
C4—C3—C2	116.5 (5)	N1^{ii}—Ni1—O1^{ii}	90.7 (2)
C4—C3—C6	124.0 (5)	N1—Ni1—O1^{ii}	89.3 (2)
C2—C3—C6	119.5 (5)	O2—Ni1—O1	94.1 (3)
C5—C4—C3	120.1 (5)	O2^{ii}—Ni1—O1	85.9 (3)
C5—C4—H4	119.9	N1^{ii}—Ni1—O1	89.3 (2)
C3—C4—H4	119.9	N1—Ni1—O1	90.7 (2)
N1—C5—C4	123.9 (6)	O1^{ii}—Ni1—O1	179.999 (2)
N1—C5—H5	118.1	Ni1—O1—H1A	119 (6)

C4—C5—H5	118.1	Ni1—O1—H1B	96 (6)
C6^{i}—C6—C3	124.7 (7)	H1A—O1—H1B	102 (8)
C6^{i}—C6—H6	117.7	Ni1—O2—H2A	118 (5)
C3—C6—H6	117.7	Ni1—O2—H2B	108 (5)
C1—N1—C5	116.5 (5)	H2A—O2—H2B	112 (9)
C1—N1—Ni1	123.9 (4)	O5—N2—O4	120.8 (6)
C5—N1—Ni1	119.6 (4)	O5—N2—O3	120.0 (6)
O2—Ni1—O2^{ii}	180.0	O4—N2—O3	119.3 (5)
O2—Ni1—N1^{ii}	89.95 (18)		

N1—C1—C2—C3	0.7 (12)	C4—C5—N1—C1	4.3 (10)
C1—C2—C3—C4	2.2 (11)	C4—C5—N1—Ni1	−176.6 (6)
C1—C2—C3—C6	−178.6 (7)	C1—N1—Ni1—O2	−134.3 (5)
C2—C3—C4—C5	−1.8 (11)	C5—N1—Ni1—O2	46.7 (5)
C6—C3—C4—C5	179.1 (7)	C1—N1—Ni1—O2^{ii}	45.7 (5)
C3—C4—C5—N1	−1.5 (11)	C5—N1—Ni1—O2^{ii}	−133.3 (5)
C4—C3—C6—C6^{i}	−9.6 (17)	C1—N1—Ni1—O1^{ii}	−48.4 (5)
C2—C3—C6—C6^{i}	171.3 (11)	C5—N1—Ni1—O1^{ii}	132.5 (5)
C2—C1—N1—C5	−3.8 (10)	C1—N1—Ni1—O1	131.6 (5)
C2—C1—N1—Ni1	177.1 (6)	C5—N1—Ni1—O1	−47.5 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*B*···O3^{iii}	0.93 (7)	2.28 (8)	3.176 (9)	162 (8)
O2—H2*A*···O5^{iv}	0.93 (6)	2.14 (7)	3.068 (8)	176 (7)
O1—H1*B*···O3^{v}	0.93 (4)	2.29 (2)	3.212 (9)	170 (8)
O1—H1*A*···O4^{vi}	0.93 (6)	2.37 (3)	3.252 (8)	158 (7)

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