Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aquabis(but-2-enoato-κO)(di-2-pyridylamine-$\kappa^2 N,N'$)nickel(II)

Jian Yu* and Ling Zhang

Department of Chemistry, Lishui College, 323000 Lishui, Zhejiang, People's Republic of China
Correspondence e-mail: zjls01@126.com

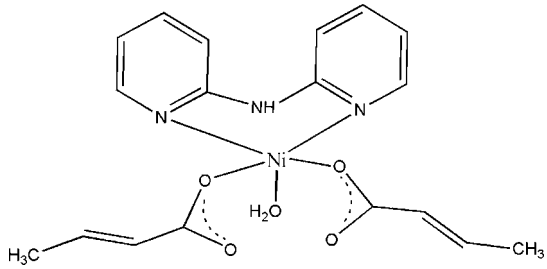
Received 6 October 2007; accepted 7 October 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.086; data-to-parameter ratio = 10.5.

In the title complex, $[Ni(C_4H_5O_2)_2(C_{10}H_9N_3)(H_2O)]$, the Ni atom adopts a square-pyramidal NiO_3N_2 geometry, with the water molecule at the apical position and N_2O_2 donors in the basal plane. A network of O—H···O and N—H···O hydrogen bonds helps to establish the packing.

Related literature

For background, see: Yang *et al.* (1997).



Experimental

Crystal data

$[Ni(C_4H_5O_2)_2(C_{10}H_9N_3)(H_2O)]$
M_r = 418.09
Monoclinic, $P2_1/n$
a = 7.1113 (7) Å
b = 16.8303 (15) Å
c = 15.9850 (14) Å
β = 91.291 (2)°
V = 1912.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.05 mm^{-1}
T = 298 (2) K
0.28 × 0.20 × 0.17 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.758, T_{max} = 0.842
9697 measured reflections
3448 independent reflections
2714 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.086
S = 0.91
3448 reflections
328 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—N1	1.9965 (19)	Ni1—O1	1.9953 (17)
Ni1—N3	2.020 (2)	Ni1—O5	2.211 (3)
Ni1—O3	1.9449 (19)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H20···O4	0.860 (9)	1.776 (17)	2.581 (3)	155 (4)
O5—H21···O2^{i}	0.861 (18)	1.874 (19)	2.731 (3)	173 (3)
N2—H9···O2^{ii}	0.877 (15)	1.925 (16)	2.801 (3)	177 (2)

Symmetry codes: (i) $x+1, y, z$; (ii) $-x, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXL97*.

The authors are grateful to Lishui College for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2571).

References

Bruker (2004). *APEX2*, *SAINT*, *SADABS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Yang, M. H., Lin, T. W., Chou, C. C., Lee, H. C., Chang, H. C., Lee, G. H., Leung, M. K. & Peng, S. M. (1997). *Chem. Commun.* pp. 39–40.

  doi:10.1107/S1600536807049100

supplementary materials

Acta Cryst. (2007). E**63**, m2706 [**doi:10.1107/S1600536807049100**]

Aquabis(but-2-enoato-κO)(di-2-pyridylamine-$\kappa^2 N,N'$)nickel(II)

J. Yu and L. Zhang

Comment

The molecular title complex, (I), complements related materials (Yang *et al.*, 1997).

As shown in Fig. 1, the Ni(II) ion in (I) is coordinated by two N atoms of one chelating dipyridin-2-ylamine ligand, two O atoms of monodentate crotonictate anions and one O atom of a water molecule, forming a square-pyramidal coordination environment (Table 1). The N atoms occupy sites in the basal plane and the water molecule occupies the apical site.

A network of O—H···O and N—H···O hydrogen bonds helps to stabilize the packing (Table 2).

Experimental

Dipyridin-2-ylamine (0.031 g, 0.016 mmol), crotonictic acid (0.028 g, 0.032 mmol), $Ni(CH_3COO)_2$ (0.18 g, 0.018 mmol) and NaOH (0.048 g, 0.12 mmol), were added to a mixed solvent of ethanol and acetonitrile. The mixture was heated for five hours under reflux with stirring. The resultant filtrate was infiltrated with diethyl ether in a closed vessel, and green blocks of (I) grew after one week.

Refinement

The C-bound H atoms were located in difference maps and freely refined. The O– and N-bound H atoms were located in difference maps and refined with O—H = 0.86 (1)Å and N—H = 0.88 (1) Å, respectively.

Figures

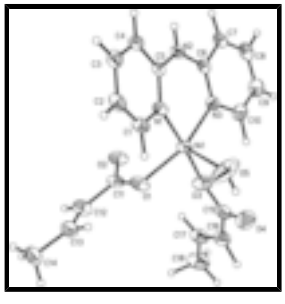


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms).

Aquabis(but-2-enoato-κ*O*)(di-2-pyridylamine-$\kappa^2 N,N'$)nickel(II)

Crystal data

$[Ni(C_4H_5O_2)_2(C_{10}H_9N_3)(H_2O)]$ $F_{000} = 872$

M_r = 418.09	D_x = 1.452 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3448 reflections
a = 7.1113 (7) Å	θ = 1.8–25.2º
b = 16.8303 (15) Å	μ = 1.05 mm^{-1}
c = 15.9850 (14) Å	T = 298 (2) K
β = 91.291 (2)º	Block, green
V = 1912.7 (3) Å^3	0.28 × 0.20 × 0.17 mm
Z = 4	

Data collection

Bruker APEXII CCD diffractometer	3448 independent reflections
Radiation source: fine-focus sealed tube	2714 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.064
T = 298(2) K	θ_{max} = 25.2º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Bruker, 2004)	h = −7→8
T_{min} = 0.758, T_{max} = 0.842	k = −20→20
9697 measured reflections	l = −17→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.037	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.086	$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2 + 0.001P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.91	$(\Delta/\sigma)_{max}$ = 0.001
3448 reflections	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
328 parameters	$\Delta\rho_{min}$ = −0.33 e Å^{-3}
4 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	0.19266 (4)	0.572833 (16)	0.669656 (17)	0.04340 (13)
O1	0.0960 (3)	0.68412 (10)	0.67000 (11)	0.0608 (5)
O2	−0.1803 (3)	0.62915 (11)	0.64370 (12)	0.0671 (5)
O3	0.0968 (3)	0.56323 (11)	0.78220 (12)	0.0723 (6)
O4	0.3460 (4)	0.59215 (14)	0.86344 (14)	0.0888 (7)
O5	0.4813 (4)	0.6002 (2)	0.71520 (16)	0.1188 (10)
N1	0.2755 (3)	0.58874 (10)	0.55233 (12)	0.0433 (5)
N2	0.2024 (3)	0.45996 (11)	0.50416 (12)	0.0449 (5)
N3	0.1835 (3)	0.45412 (12)	0.65126 (12)	0.0468 (5)
C1	0.3433 (4)	0.66180 (14)	0.53393 (17)	0.0514 (6)
C2	0.3911 (4)	0.68475 (16)	0.45623 (17)	0.0563 (7)
C3	0.3701 (4)	0.63070 (15)	0.39151 (17)	0.0560 (7)
C4	0.3075 (4)	0.55611 (15)	0.40780 (16)	0.0495 (6)
C5	0.2626 (3)	0.53616 (13)	0.48997 (14)	0.0399 (5)
C6	0.1751 (3)	0.41812 (12)	0.57651 (15)	0.0427 (6)
C7	0.1412 (4)	0.33687 (14)	0.56819 (18)	0.0536 (7)
C8	0.1230 (4)	0.29112 (17)	0.6374 (2)	0.0666 (8)
C9	0.1385 (5)	0.32646 (18)	0.7143 (2)	0.0741 (9)
C10	0.1671 (5)	0.40643 (17)	0.71917 (18)	0.0658 (8)
C11	−0.0792 (4)	0.68798 (15)	0.65862 (15)	0.0538 (6)
C12	−0.1703 (5)	0.76715 (19)	0.6610 (2)	0.0725 (9)
C13	−0.0853 (6)	0.83326 (18)	0.65710 (19)	0.0694 (8)
C14	−0.1754 (8)	0.9141 (2)	0.6553 (3)	0.0914 (12)
C15	0.1761 (5)	0.58259 (14)	0.85134 (18)	0.0604 (8)
C16	0.0516 (6)	0.59262 (17)	0.9241 (2)	0.0715 (9)
C17	−0.1283 (6)	0.59352 (17)	0.9198 (2)	0.0746 (9)
C18	−0.2552 (8)	0.6050 (3)	0.9942 (3)	0.1003 (13)
H9	0.195 (3)	0.4304 (11)	0.4590 (11)	0.044 (7)*
H1	0.356 (3)	0.6974 (14)	0.5834 (16)	0.060 (7)*
H4	0.292 (4)	0.5178 (16)	0.3622 (17)	0.070 (8)*
H3	0.398 (4)	0.6468 (13)	0.3352 (15)	0.054 (7)*
H19	−0.161 (5)	0.6191 (18)	1.047 (2)	0.092 (11)*
H6	0.098 (4)	0.2320 (16)	0.6302 (15)	0.068 (8)*
H2	0.437 (3)	0.7340 (15)	0.4474 (15)	0.056 (7)*
H5	0.130 (4)	0.3151 (15)	0.5107 (16)	0.062 (8)*
H15	0.100 (5)	0.6118 (19)	0.986 (2)	0.104 (11)*
H14	−0.320 (7)	0.912 (2)	0.663 (3)	0.14 (2)*
H18	−0.349 (6)	0.658 (2)	0.982 (2)	0.148 (16)*
H12	−0.149 (6)	0.940 (2)	0.602 (3)	0.133 (16)*
H8	0.179 (5)	0.4376 (17)	0.777 (2)	0.090 (10)*
H7	0.138 (4)	0.3000 (17)	0.7626 (18)	0.077 (9)*
H21	0.5918 (19)	0.610 (2)	0.6968 (19)	0.098 (11)*

H20	0.467 (6)	0.604 (2)	0.7683 (4)	0.117 (14)*
H10	−0.304 (6)	0.774 (3)	0.656 (2)	0.144 (17)*
H11	0.051 (6)	0.824 (2)	0.658 (2)	0.125 (15)*
H16	−0.186 (6)	0.587 (2)	0.864 (3)	0.142 (17)*
H17	−0.315 (6)	0.560 (2)	1.012 (3)	0.133 (17)*
H13	−0.120 (5)	0.947 (2)	0.700 (2)	0.113 (14)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0463 (2)	0.03944 (18)	0.0448 (2)	−0.00627 (13)	0.00914 (14)	−0.00722 (12)
O1	0.0586 (12)	0.0435 (10)	0.0810 (13)	−0.0096 (9)	0.0216 (10)	−0.0161 (8)
O2	0.0676 (13)	0.0583 (11)	0.0758 (13)	−0.0152 (10)	0.0092 (10)	−0.0227 (9)
O3	0.0816 (15)	0.0798 (14)	0.0563 (12)	−0.0182 (11)	0.0211 (11)	−0.0110 (10)
O4	0.0887 (18)	0.1121 (19)	0.0657 (13)	0.0090 (15)	0.0046 (13)	−0.0040 (12)
O5	0.0608 (16)	0.232 (3)	0.0634 (16)	−0.0454 (19)	0.0058 (13)	−0.0179 (18)
N1	0.0430 (12)	0.0356 (10)	0.0515 (12)	−0.0028 (8)	0.0071 (9)	−0.0044 (8)
N2	0.0556 (13)	0.0323 (10)	0.0469 (12)	−0.0020 (9)	0.0042 (10)	−0.0058 (9)
N3	0.0493 (13)	0.0411 (10)	0.0500 (12)	0.0018 (9)	0.0034 (10)	0.0044 (9)
C1	0.0549 (16)	0.0387 (13)	0.0608 (16)	−0.0069 (12)	0.0108 (13)	−0.0050 (12)
C2	0.0583 (17)	0.0379 (14)	0.0734 (19)	−0.0023 (13)	0.0145 (14)	0.0062 (13)
C3	0.0602 (17)	0.0517 (16)	0.0567 (16)	0.0042 (13)	0.0138 (14)	0.0119 (13)
C4	0.0556 (16)	0.0455 (15)	0.0477 (15)	0.0031 (12)	0.0064 (12)	−0.0032 (12)
C5	0.0356 (12)	0.0325 (11)	0.0518 (14)	0.0026 (10)	0.0043 (10)	−0.0008 (10)
C6	0.0366 (13)	0.0358 (12)	0.0559 (15)	0.0004 (10)	0.0039 (11)	0.0022 (11)
C7	0.0565 (17)	0.0365 (13)	0.0679 (18)	−0.0009 (12)	0.0037 (14)	−0.0009 (12)
C8	0.0668 (19)	0.0420 (16)	0.091 (2)	0.0006 (14)	0.0043 (16)	0.0139 (15)
C9	0.093 (3)	0.0577 (19)	0.072 (2)	−0.0030 (16)	0.0045 (18)	0.0257 (17)
C10	0.084 (2)	0.0581 (17)	0.0552 (17)	−0.0019 (15)	0.0033 (15)	0.0114 (14)
C11	0.0607 (18)	0.0491 (15)	0.0523 (15)	−0.0026 (14)	0.0159 (13)	−0.0137 (12)
C12	0.068 (2)	0.0622 (19)	0.088 (2)	0.0017 (17)	0.0144 (18)	−0.0167 (16)
C13	0.088 (3)	0.0544 (18)	0.0661 (19)	0.0018 (18)	0.0069 (17)	−0.0039 (14)
C14	0.127 (4)	0.056 (2)	0.092 (3)	0.021 (2)	0.007 (3)	0.003 (2)
C15	0.089 (2)	0.0418 (15)	0.0513 (17)	0.0103 (15)	0.0145 (16)	0.0011 (12)
C16	0.098 (3)	0.0581 (18)	0.0585 (19)	0.0079 (18)	0.0128 (18)	−0.0005 (14)
C17	0.095 (3)	0.0511 (17)	0.079 (2)	−0.0052 (18)	0.021 (2)	−0.0035 (15)
C18	0.117 (4)	0.088 (3)	0.098 (3)	−0.006 (3)	0.050 (3)	−0.010 (2)

Geometric parameters (Å, °)

Ni1—N1	1.9965 (19)	C4—H4	0.98 (3)
Ni1—N3	2.020 (2)	C6—C7	1.394 (3)
Ni1—O3	1.9449 (19)	C7—C8	1.357 (4)
Ni1—O1	1.9953 (17)	C7—H5	0.99 (3)
Ni1—O5	2.211 (3)	C8—C9	1.367 (4)
O1—C11	1.257 (3)	C8—H6	1.02 (3)
O2—C11	1.243 (3)	C9—C10	1.363 (4)
O3—C15	1.272 (4)	C9—H7	0.89 (3)
O4—C15	1.230 (4)	C10—H8	1.06 (3)

O5—H21	0.864 (18)	C11—C12	1.482 (4)
O5—H20	0.860 (9)	C12—C13	1.268 (4)
N1—C5	1.335 (3)	C12—H10	0.96 (4)
N1—C1	1.355 (3)	C13—C14	1.505 (5)
N2—C6	1.372 (3)	C13—H11	0.99 (4)
N2—C5	1.373 (3)	C14—H14	1.04 (5)
N2—H9	0.877 (15)	C14—H12	0.97 (4)
N3—C6	1.340 (3)	C14—H13	0.98 (4)
N3—C10	1.357 (3)	C15—C16	1.486 (4)
C1—C2	1.351 (4)	C16—C17	1.280 (5)
C1—H1	0.99 (3)	C16—H15	1.08 (3)
C2—C3	1.383 (4)	C17—C18	1.522 (5)
C2—H2	0.90 (2)	C17—H16	0.98 (4)
C3—C4	1.359 (3)	C18—H19	1.09 (3)
C3—H3	0.97 (2)	C18—H18	1.13 (4)
C4—C5	1.400 (3)	C18—H17	0.92 (4)
O3—Ni1—O1	86.99 (8)	C8—C7—C6	119.9 (3)
O3—Ni1—N1	175.62 (8)	C8—C7—H5	122.6 (15)
O1—Ni1—N1	89.18 (7)	C6—C7—H5	117.5 (15)
O3—Ni1—N3	92.38 (8)	C7—C8—C9	118.6 (3)
O1—Ni1—N3	156.74 (8)	C7—C8—H6	118.9 (14)
N1—Ni1—N3	90.30 (7)	C9—C8—H6	122.5 (14)
O3—Ni1—O5	93.14 (9)	C8—C9—C10	119.3 (3)
O1—Ni1—O5	96.93 (12)	C8—C9—H7	124.0 (19)
N1—Ni1—O5	89.42 (9)	C10—C9—H7	116.6 (19)
N3—Ni1—O5	106.32 (11)	N3—C10—C9	123.6 (3)
C11—O1—Ni1	112.88 (16)	N3—C10—H8	113.4 (16)
C15—O3—Ni1	128.7 (2)	C9—C10—H8	123.0 (16)
Ni1—O5—H21	141 (2)	O2—C11—O1	123.6 (2)
Ni1—O5—H20	102 (3)	O2—C11—C12	118.0 (3)
H21—O5—H20	117 (3)	O1—C11—C12	118.4 (3)
C5—N1—C1	117.3 (2)	C13—C12—C11	125.4 (3)
C5—N1—Ni1	126.58 (15)	C13—C12—H10	111 (3)
C1—N1—Ni1	116.07 (15)	C11—C12—H10	123 (3)
C6—N2—C5	132.0 (2)	C12—C13—C14	126.3 (4)
C6—N2—H9	113.3 (14)	C12—C13—H11	109 (2)
C5—N2—H9	114.1 (14)	C14—C13—H11	125 (2)
C6—N3—C10	116.3 (2)	C13—C14—H14	113 (2)
C6—N3—Ni1	125.28 (16)	C13—C14—H12	109 (2)
C10—N3—Ni1	118.14 (19)	H14—C14—H12	110 (3)
C2—C1—N1	123.8 (2)	C13—C14—H13	109 (2)
C2—C1—H1	122.5 (14)	H14—C14—H13	108 (3)
N1—C1—H1	113.7 (14)	H12—C14—H13	108 (3)
C1—C2—C3	118.3 (2)	O4—C15—O3	125.8 (3)
C1—C2—H2	120.4 (16)	O4—C15—C16	117.5 (3)
C3—C2—H2	121.3 (16)	O3—C15—C16	116.7 (3)
C4—C3—C2	119.6 (2)	C17—C16—C15	124.8 (3)
C4—C3—H3	121.0 (14)	C17—C16—H15	109.8 (18)
C2—C3—H3	119.4 (14)	C15—C16—H15	124.3 (19)

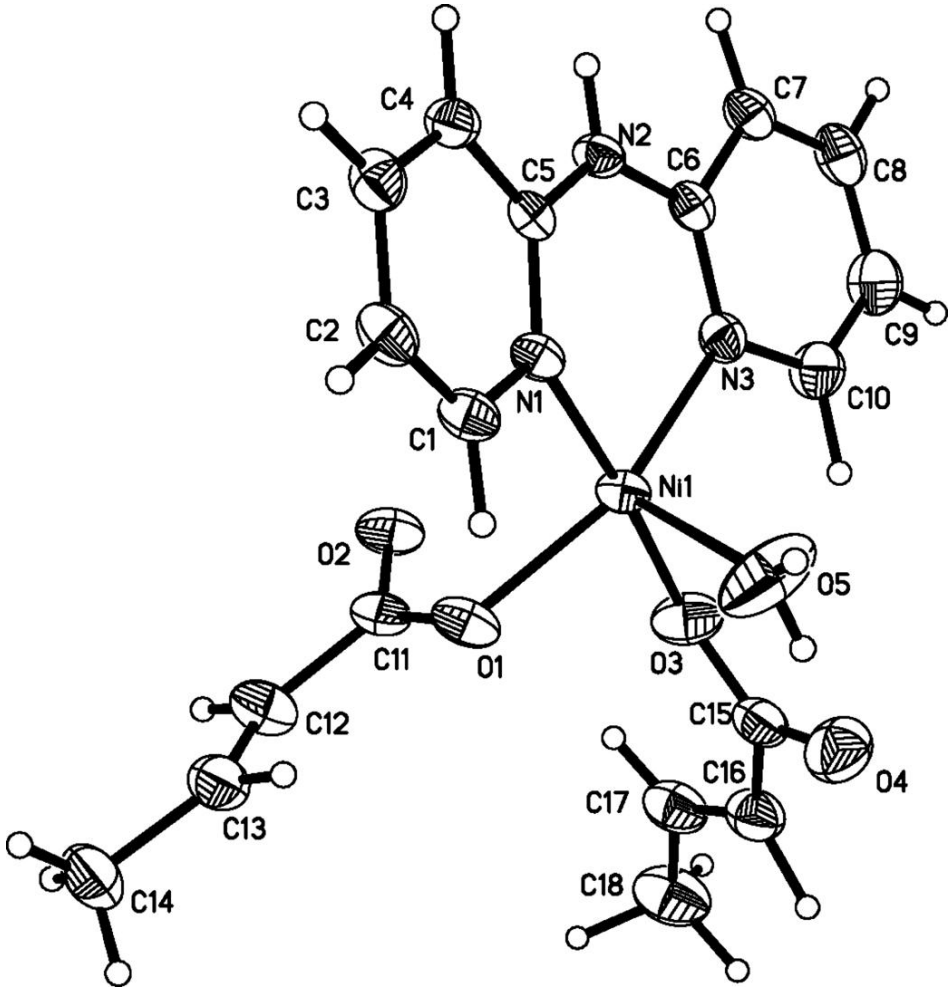
C3—C4—C5	118.9 (2)	C16—C17—C18	124.7 (4)
C3—C4—H4	119.8 (16)	C16—C17—H16	117 (3)
C5—C4—H4	121.2 (16)	C18—C17—H16	119 (3)
N1—C5—N2	120.8 (2)	C17—C18—H19	105.4 (18)
N1—C5—C4	121.9 (2)	C17—C18—H18	109 (2)
N2—C5—C4	117.2 (2)	H19—C18—H18	108 (3)
N3—C6—N2	121.0 (2)	C17—C18—H17	116 (3)
N3—C6—C7	122.2 (2)	H19—C18—H17	103 (3)
N2—C6—C7	116.8 (2)	H18—C18—H17	115 (4)
O3—Ni1—O1—C11	−76.91 (18)	Ni1—N1—C5—C4	173.39 (18)
N1—Ni1—O1—C11	100.97 (18)	C6—N2—C5—N1	−11.9 (4)
N3—Ni1—O1—C11	12.1 (3)	C6—N2—C5—C4	168.7 (2)
O5—Ni1—O1—C11	−169.71 (18)	C3—C4—C5—N1	1.5 (4)
O1—Ni1—O3—C15	−85.3 (2)	C3—C4—C5—N2	−179.1 (2)
O5—Ni1—O3—C15	11.5 (2)	C10—N3—C6—N2	−175.7 (2)
O1—Ni1—N1—C5	−140.0 (2)	Ni1—N3—C6—N2	10.6 (3)
N3—Ni1—N1—C5	16.7 (2)	C10—N3—C6—C7	3.4 (4)
O5—Ni1—N1—C5	123.1 (2)	Ni1—N3—C6—C7	−170.30 (19)
O1—Ni1—N1—C1	36.66 (19)	C5—N2—C6—N3	9.3 (4)
N3—Ni1—N1—C1	−166.59 (19)	C5—N2—C6—C7	−169.9 (2)
O5—Ni1—N1—C1	−60.3 (2)	N3—C6—C7—C8	−2.7 (4)
O3—Ni1—N3—C6	157.6 (2)	N2—C6—C7—C8	176.5 (3)
O1—Ni1—N3—C6	69.7 (3)	C6—C7—C8—C9	0.0 (5)
N1—Ni1—N3—C6	−18.9 (2)	C7—C8—C9—C10	1.6 (5)
O5—Ni1—N3—C6	−108.4 (2)	C6—N3—C10—C9	−1.7 (4)
O3—Ni1—N3—C10	−16.0 (2)	Ni1—N3—C10—C9	172.4 (3)
O1—Ni1—N3—C10	−103.9 (3)	C8—C9—C10—N3	−0.8 (5)
N1—Ni1—N3—C10	167.4 (2)	Ni1—O1—C11—O2	−4.1 (3)
O5—Ni1—N3—C10	78.0 (2)	Ni1—O1—C11—C12	177.52 (19)
C5—N1—C1—C2	2.6 (4)	O2—C11—C12—C13	−163.8 (3)
Ni1—N1—C1—C2	−174.4 (2)	O1—C11—C12—C13	14.7 (5)
N1—C1—C2—C3	−0.1 (4)	C11—C12—C13—C14	176.9 (3)
C1—C2—C3—C4	−1.8 (4)	Ni1—O3—C15—O4	−20.2 (4)
C2—C3—C4—C5	1.1 (4)	Ni1—O3—C15—C16	161.29 (19)
C1—N1—C5—N2	177.4 (2)	O4—C15—C16—C17	171.7 (3)
Ni1—N1—C5—N2	−5.9 (3)	O3—C15—C16—C17	−9.6 (4)
C1—N1—C5—C4	−3.2 (4)	C15—C16—C17—C18	−179.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H20···O4	0.860 (9)	1.776 (17)	2.581 (3)	155 (4)
O5—H21···O2^{i}	0.861 (18)	1.874 (19)	2.731 (3)	173 (3)
N2—H9···O2^{ii}	0.877 (15)	1.925 (16)	2.801 (3)	177 (2)

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

Fig. 1


C4
C7
N2
C5
C6
C8
C3
C2
C9
N3
N1
C10
C1
Ni1
O2
O5
C11
O1
O3
C12
C15
C16
O4
C17
C13
C18
C14