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Aquabis(4-methylbenzoato)-κO;$\kappa^2 O,O'$-bis(pyridine-κN)nickel(II)

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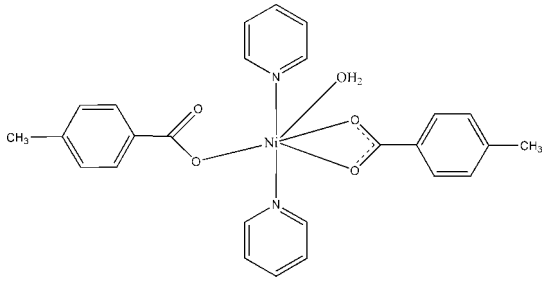
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.028; wR factor = 0.065; data-to-parameter ratio = 16.2.

In the title mononuclear complex, $[Ni(C_8H_7O_2)_2(C_5H_5N)_2(H_2O)]$, the Ni^{II} atom is in a distorted octahedral arrangement, coordinated by three carboxylate O atoms from one bidentate 4-methylbenzoate ligand and one monodentate 4-methylbenzoate ligand, two N atoms from pyridine ligands, axially positioned, and a water molecule. The equatorially positioned water molecule and uncoordinated carboxylate O atom form an intramolecular hydrogen bond. An intermolecular O—H···O hydrogen bond between the coordinated water molecule and carboxylate O atom of the 4-methylbenzoate ligand forms infinite chains along the b axis. These chains are connected by C—H···π interactions.

Related literature

For related literature, see: Song *et al.* (2007).



Experimental

Crystal data

$[Ni(C_8H_7O_2)_2(C_5H_5N)_2(H_2O)]$
M_r = 505.20
Monoclinic, $P2_1$
a = 13.6181 (1) Å
b = 5.9526 (1) Å
c = 15.1380 (2) Å
β = 107.215 (1)°
V = 1172.16 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 296 (2) K
0.26 × 0.23 × 0.20 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.806, T_{max} = 0.846
11325 measured reflections
5102 independent reflections
4798 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.065
S = 1.03
5102 reflections
315 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter: 0.00

Table 1
Selected geometric parameters (Å, °).

N1—Ni1	2.0941 (17)	Ni1—O1*W*	2.0412 (15)
N2—Ni1	2.0981 (16)	Ni1—O2	2.1107 (12)
Ni1—O3	2.0165 (14)	Ni1—O1	2.1710 (15)
O3—Ni1—O1*W*	94.41 (6)	N1—Ni1—O2	89.57 (6)
O3—Ni1—N1	86.71 (6)	N2—Ni1—O2	93.83 (6)
O1*W*—Ni1—N1	89.53 (6)	O3—Ni1—O1	104.00 (6)
O3—Ni1—N2	89.22 (6)	O1*W*—Ni1—O1	161.59 (5)
O1*W*—Ni1—N2	92.99 (6)	N1—Ni1—O1	91.67 (6)
N1—Ni1—N2	175.36 (7)	N2—Ni1—O1	87.17 (6)
O3—Ni1—O2	165.26 (7)	O2—Ni1—O1	61.82 (7)
O1*W*—Ni1—O2	99.83 (8)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H2*W*···O4	0.819 (9)	1.834 (13)	2.587 (2)	152 (2)
O1*W*—H1*W*···O1^{i}	0.809 (9)	1.957 (12)	2.739 (2)	162 (2)

Symmetry code: (i) $x, y+1, z$.

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: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* and *XP* in *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2154).

References

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Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Song, W.-D., Gu, C.-S., Hao, X.-M. & Liu, J.-W. (2007). *Acta Cryst.* E**63**, m1023–m1024.

supporting information

Acta Cryst. (2008). E**64**, m548 [doi:10.1107/S160053680800634X]

Aquabis(4-methylbenzoato)-$\kappa O;\kappa^2 O,O'$-bis(pyridine-κN)nickel(II)

Wen-Dong Song, Hao Wang and Li-Li Ji

S1. Comment

In the structural investigation of 4-methylbenzoate complexes, it has been found that the 4-methylbenzoic acid functions as a multidentate ligand [Song *et al.* (2007)] with versatile binding and coordination modes. In this paper, we report the crystal structure of the title compound, (I), a new Ni complex obtained by the reaction of 4-methylbenzoic acid, pyridine and nickel chloride in alkaline aqueous solution.

The Ni^{II} atom exhibits a disordered octahedral environment (Fig. 1, Table 1) defined by three carboxyl O atoms from one bidentate 4-methylbenzoate ligand and one monodentate 4-methylbenzoate ligand, two N atoms from two pyridine ligands and a water molecule. The intermolecular O—H···O hydrogen bond (Table 2, Fig. 2) between the coordinated water molecule and carboxy O atom of 4-methylbenzoate ligand generates a chain along the axis b. The intermolecular hydrogen bond C1—H1···O also involves water molecule [3.339 (3) %A, 145%]. An intramolecular hydrogen bond connects the coordinated water molecule and uncoordinated oxygen atom O4 (Table 2). C—H···π interactions connect hydrogen bonded chains: C_3– H_3···C_g (C_{12}→ C_{17}, symmetry code: -2 - *x*, 1/2 + *y*, 2 - *z*) of 3.482 (2) %A; 132%, and C_{14}–H14···C_g(C_{12}→ C_{17}, symmetry code: 1 - *x*, -1/2 + *y*, 2 - *z*) of 3.603 (2) %A; 134%; C_{22}– H22···C_g(C_{20}→ C_{25}, symmetry code: 2 - *x*, -1/2 + *y*, 1 - *z*) of 3.504 (2) %A; 133%.

S2. Experimental

A mixture of nickel chloride (1 mmol), 4-methylbenzoic acid (1 mmol), pyridine(1 mmol), NaOH (1.5 mmol) and H_2O (12 ml) were placed into a 23 ml Teflon reactor, which was heated to 433 K for three days and then cooled to room temperature at a rate of 10 K h^{-1}. The crystals obtained were washed with water and dryed in air.

S3. Refinement

Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.93 Å for aromatic rings, C—H = 0.96 Å for methyl group, and with U_{iso}(H) = 1.2 U_{eq}(C). Water H atoms were tentatively located in difference Fourier maps and were refined with distance restraints of O–H = 0.82 Å and H···H = 1.29 Å, each within a standard deviation of 0.01 Å; and with U_{iso}(H) = 1.5 U_{eq}(O).

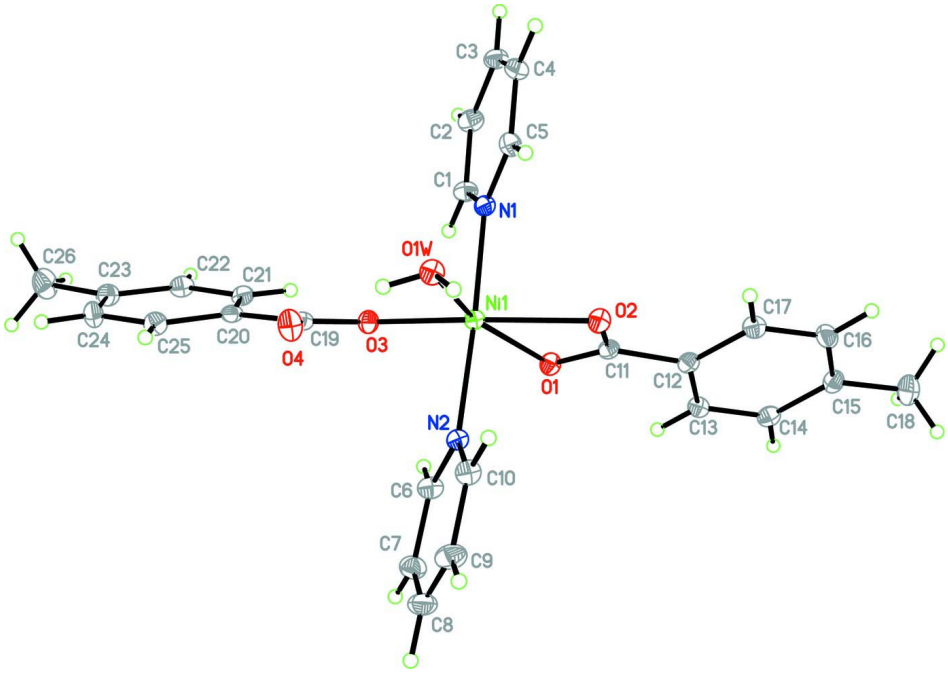

Figure 1

The structure of (I) showing the atomic numbering scheme and octahedral coordination of Ni^{II}. Non-H atoms are shown with the 30% probability displacement ellipsoids.

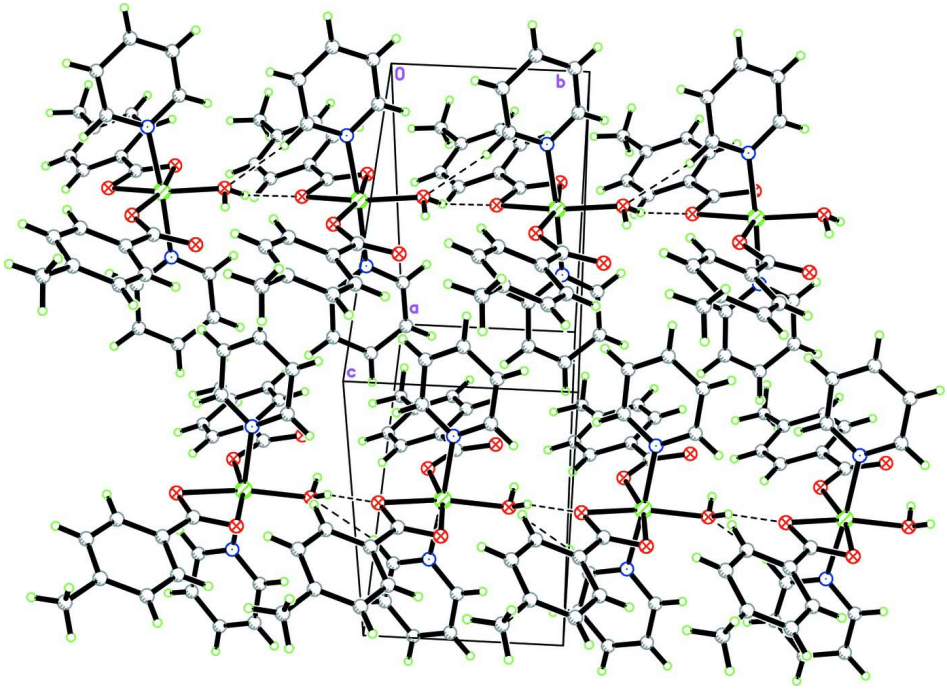

Figure 2

The crystal packing of (I). The intermolecluar hydrogen bonds are shown as dashed lines.

Aquabis(4-methylbenzoato)-$\kappa O;\kappa^2 O,O'$-bis(pyridine- κN)nickel(II)

Crystal data

$[Ni(C_8H_7O_2)_2(C_5H_5N)_2(H_2O)]$
$M_r = 505.20$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 13.6181$ (1) Å
$b = 5.9526$ (1) Å
$c = 15.1380$ (2) Å
$\beta = 107.215$ (1)°
$V = 1172.16$ (3) Å^3
$Z = 2$
$F(000) = 528$
$D_x = 1.431$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4520 reflections
$\theta = 1.4$–28°
$\mu = 0.87$ mm^{-1}
$T = 296$ K
Block, blue
0.26 × 0.23 × 0.20 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.806$, $T_{max} = 0.846$
11325 measured reflections
5102 independent reflections
4798 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.6°$
$h = -17 \rightarrow 17$
$k = -7 \rightarrow 7$
$l = -19 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.065$
$S = 1.04$
5102 reflections
315 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
$w = 1/[\sigma^2(F_o^2) + (0.0307P)^2 + 0.1736P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: 0.00

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}
C1	0.95095 (15)	0.1169 (4)	0.82231 (15)	0.0247 (4)
H1	0.9142	0.0108	0.7803	0.030*
C2	1.05343 (16)	0.0757 (4)	0.86802 (16)	0.0296 (5)

H2	1.0845	−0.0563	0.8571	0.036*
C3	1.10915 (16)	0.2322 (4)	0.92999 (16)	0.0305 (5)
H3	1.1782	0.2083	0.9613	0.037*
C4	1.06002 (16)	0.4243 (4)	0.94418 (15)	0.0292 (5)
H4	1.0954	0.5331	0.9855	0.035*
C5	0.95739 (16)	0.4540 (4)	0.89642 (15)	0.0261 (5)
H5	0.9250	0.5847	0.9067	0.031*
C6	0.55162 (16)	0.2440 (4)	0.62678 (16)	0.0272 (5)
H6	0.5903	0.1158	0.6259	0.033*
C7	0.45288 (17)	0.2553 (4)	0.56751 (17)	0.0322 (5)
H7	0.4258	0.1367	0.5278	0.039*
C8	0.39535 (17)	0.4435 (4)	0.56807 (18)	0.0352 (6)
H8	0.3286	0.4545	0.5288	0.042*
C9	0.43788 (17)	0.6170 (4)	0.62781 (17)	0.0345 (5)
H9	0.4004	0.7468	0.6292	0.041*
C10	0.53759 (16)	0.5937 (4)	0.68568 (15)	0.0273 (5)
H10	0.5661	0.7104	0.7260	0.033*
C11	0.69445 (14)	0.1687 (3)	0.88686 (14)	0.0200 (4)
C12	0.66663 (15)	0.0548 (4)	0.96375 (14)	0.0214 (4)
C13	0.62152 (14)	−0.1580 (4)	0.95154 (13)	0.0227 (4)
H13	0.6066	−0.2280	0.8941	0.027*
C14	0.59873 (15)	−0.2661 (4)	1.02416 (15)	0.0257 (5)
H14	0.5669	−0.4059	1.0143	0.031*
C15	0.62267 (15)	−0.1690 (4)	1.11155 (14)	0.0263 (5)
C16	0.66774 (16)	0.0436 (4)	1.12359 (15)	0.0289 (5)
H16	0.6843	0.1115	1.1815	0.035*
C17	0.68834 (16)	0.1557 (4)	1.05043 (15)	0.0252 (4)
H17	0.7168	0.2990	1.0594	0.030*
C18	0.6011 (2)	−0.2912 (5)	1.19129 (17)	0.0405 (6)
H18A	0.6522	−0.2515	1.2479	0.061*
H18B	0.6030	−0.4503	1.1816	0.061*
H18C	0.5343	−0.2494	1.1950	0.061*
C19	0.78596 (14)	0.4041 (4)	0.58580 (14)	0.0216 (5)
C20	0.82429 (14)	0.3106 (3)	0.50984 (14)	0.0209 (5)
C21	0.87038 (15)	0.0988 (4)	0.51907 (15)	0.0237 (4)
H21	0.8747	0.0125	0.5713	0.028*
C22	0.90959 (16)	0.0170 (4)	0.45091 (15)	0.0258 (5)
H22	0.9409	−0.1235	0.4584	0.031*
C23	0.90311 (16)	0.1405 (4)	0.37128 (15)	0.0285 (5)
C24	0.85529 (15)	0.3503 (5)	0.36190 (13)	0.0294 (4)
H24	0.8491	0.4350	0.3089	0.035*
C25	0.81695 (16)	0.4341 (4)	0.43050 (15)	0.0258 (5)
H25	0.7859	0.5748	0.4232	0.031*
C26	0.9479 (2)	0.0517 (5)	0.29837 (16)	0.0423 (6)
H26A	0.8973	0.0607	0.2389	0.063*
H26B	0.9682	−0.1020	0.3118	0.063*
H26C	1.0068	0.1398	0.2980	0.063*
N1	0.90261 (12)	0.3038 (3)	0.83626 (12)	0.0219 (4)

N2	0.59440 (12)	0.4102 (3)	0.68585 (12)	0.0213 (4)
Ni1	0.748180 (17)	0.36693 (5)	0.764977 (16)	0.01841 (7)
O1	0.69972 (10)	0.0586 (2)	0.81637 (9)	0.0226 (3)
O2	0.71436 (10)	0.3781 (4)	0.89227 (9)	0.0241 (3)
O3	0.78210 (11)	0.2707 (2)	0.64966 (10)	0.0232 (3)
O4	0.76152 (12)	0.6085 (3)	0.58101 (10)	0.0310 (4)
O1W	0.78338 (11)	0.6967 (2)	0.75308 (10)	0.0245 (3)
H2W	0.7754 (18)	0.715 (4)	0.6978 (7)	0.037*
H1W	0.7470 (16)	0.789 (3)	0.7669 (14)	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0227 (10)	0.0198 (10)	0.0305 (11)	−0.0009 (9)	0.0060 (9)	−0.0009 (9)
C2	0.0248 (11)	0.0261 (12)	0.0374 (13)	0.0035 (10)	0.0083 (9)	0.0022 (10)
C3	0.0191 (10)	0.0396 (14)	0.0307 (12)	−0.0009 (10)	0.0041 (9)	0.0063 (11)
C4	0.0276 (10)	0.0332 (15)	0.0241 (11)	−0.0077 (9)	0.0036 (9)	−0.0048 (9)
C5	0.0287 (11)	0.0266 (11)	0.0232 (11)	0.0003 (9)	0.0079 (9)	−0.0019 (8)
C6	0.0235 (10)	0.0251 (12)	0.0319 (12)	0.0003 (9)	0.0066 (9)	−0.0033 (10)
C7	0.0285 (12)	0.0341 (13)	0.0308 (13)	−0.0050 (11)	0.0038 (10)	−0.0029 (10)
C8	0.0218 (10)	0.0407 (14)	0.0387 (14)	−0.0009 (10)	0.0021 (10)	0.0098 (10)
C9	0.0245 (11)	0.0316 (13)	0.0466 (15)	0.0077 (10)	0.0092 (10)	0.0048 (11)
C10	0.0279 (11)	0.0249 (11)	0.0293 (11)	0.0008 (9)	0.0087 (9)	−0.0014 (9)
C11	0.0161 (9)	0.0205 (11)	0.0235 (10)	0.0041 (8)	0.0061 (8)	0.0006 (8)
C12	0.0189 (9)	0.0206 (11)	0.0253 (10)	0.0048 (8)	0.0075 (8)	0.0004 (9)
C13	0.0230 (8)	0.0204 (12)	0.0239 (9)	0.0016 (9)	0.0056 (7)	−0.0027 (10)
C14	0.0229 (10)	0.0232 (11)	0.0316 (12)	−0.0011 (9)	0.0089 (9)	−0.0001 (9)
C15	0.0252 (9)	0.0285 (15)	0.0271 (10)	0.0042 (9)	0.0108 (8)	0.0047 (10)
C16	0.0294 (11)	0.0341 (13)	0.0224 (11)	0.0022 (10)	0.0067 (9)	−0.0055 (10)
C17	0.0251 (10)	0.0218 (11)	0.0284 (11)	0.0000 (9)	0.0076 (9)	−0.0040 (9)
C18	0.0501 (15)	0.0426 (15)	0.0337 (14)	0.0007 (13)	0.0202 (12)	0.0064 (12)
C19	0.0159 (8)	0.0243 (15)	0.0230 (10)	0.0013 (9)	0.0032 (7)	−0.0002 (9)
C20	0.0156 (8)	0.0236 (12)	0.0222 (10)	−0.0017 (7)	0.0037 (7)	−0.0029 (8)
C21	0.0202 (9)	0.0229 (11)	0.0275 (11)	0.0000 (9)	0.0065 (8)	0.0020 (9)
C22	0.0231 (10)	0.0220 (11)	0.0327 (12)	0.0028 (9)	0.0089 (9)	−0.0038 (10)
C23	0.0258 (10)	0.0332 (13)	0.0272 (11)	−0.0001 (9)	0.0090 (9)	−0.0065 (10)
C24	0.0350 (10)	0.0332 (12)	0.0216 (9)	0.0018 (13)	0.0106 (8)	0.0035 (13)
C25	0.0258 (10)	0.0223 (11)	0.0290 (11)	0.0034 (8)	0.0076 (9)	0.0018 (8)
C26	0.0485 (15)	0.0510 (17)	0.0313 (13)	0.0134 (13)	0.0177 (11)	−0.0049 (13)
N1	0.0202 (8)	0.0233 (10)	0.0221 (8)	−0.0003 (6)	0.0061 (7)	0.0014 (7)
N2	0.0198 (7)	0.0215 (12)	0.0228 (8)	−0.0004 (7)	0.0066 (6)	−0.0004 (7)
Ni1	0.01837 (11)	0.01668 (11)	0.02025 (11)	0.00073 (12)	0.00583 (8)	−0.00085 (14)
O1	0.0258 (7)	0.0196 (7)	0.0244 (7)	0.0010 (6)	0.0103 (6)	−0.0028 (6)
O2	0.0285 (6)	0.0193 (7)	0.0264 (7)	−0.0009 (9)	0.0110 (5)	−0.0020 (9)
O3	0.0260 (7)	0.0231 (7)	0.0221 (8)	0.0015 (6)	0.0097 (6)	−0.0011 (6)
O4	0.0437 (9)	0.0232 (8)	0.0288 (8)	0.0098 (7)	0.0151 (7)	0.0014 (7)
O1W	0.0283 (7)	0.0186 (8)	0.0274 (8)	0.0013 (6)	0.0097 (6)	−0.0031 (7)

Geometric parameters (Å, º)

C1—N1	1.341 (3)	C15—C18	1.511 (3)
C1—C2	1.384 (3)	C16—C17	1.391 (3)
C1—H1	0.9300	C16—H16	0.9300
C2—C3	1.379 (3)	C17—H17	0.9300
C2—H2	0.9300	C18—H18A	0.9600
C3—C4	1.373 (3)	C18—H18B	0.9600
C3—H3	0.9300	C18—H18C	0.9600
C4—C5	1.382 (3)	C19—O4	1.258 (3)
C4—H4	0.9300	C19—O3	1.264 (3)
C5—N1	1.335 (3)	C19—C20	1.503 (3)
C5—H5	0.9300	C20—C25	1.386 (3)
C6—N2	1.345 (3)	C20—C21	1.396 (3)
C6—C7	1.380 (3)	C21—C22	1.383 (3)
C6—H6	0.9300	C21—H21	0.9300
C7—C8	1.369 (3)	C22—C23	1.393 (3)
C7—H7	0.9300	C22—H22	0.9300
C8—C9	1.382 (4)	C23—C24	1.396 (4)
C8—H8	0.9300	C23—C26	1.506 (3)
C9—C10	1.388 (3)	C24—C25	1.386 (3)
C9—H9	0.9300	C24—H24	0.9300
C10—N2	1.338 (3)	C25—H25	0.9300
C10—H10	0.9300	C26—H26A	0.9600
C11—O1	1.272 (2)	C26—H26B	0.9600
C11—O2	1.273 (3)	C26—H26C	0.9600
C11—C12	1.490 (3)	N1—Ni1	2.0941 (17)
C12—C17	1.393 (3)	N2—Ni1	2.0981 (16)
C12—C13	1.396 (3)	Ni1—O3	2.0165 (14)
C13—C14	1.386 (3)	Ni1—O1W	2.0412 (15)
C13—H13	0.9300	Ni1—O2	2.1107 (12)
C14—C15	1.391 (3)	Ni1—O1	2.1710 (15)
C14—H14	0.9300	O1W—H2W	0.819 (9)
C15—C16	1.395 (3)	O1W—H1W	0.809 (9)
N1—C1—C2	122.5 (2)	H18B—C18—H18C	109.5
N1—C1—H1	118.7	O4—C19—O3	125.6 (2)
C2—C1—H1	118.7	O4—C19—C20	117.39 (19)
C3—C2—C1	119.4 (2)	O3—C19—C20	117.1 (2)
C3—C2—H2	120.3	C25—C20—C21	118.70 (19)
C1—C2—H2	120.3	C25—C20—C19	120.93 (19)
C4—C3—C2	118.2 (2)	C21—C20—C19	120.35 (18)
C4—C3—H3	120.9	C22—C21—C20	120.3 (2)
C2—C3—H3	120.9	C22—C21—H21	119.8
C3—C4—C5	119.3 (2)	C20—C21—H21	119.8
C3—C4—H4	120.4	C21—C22—C23	121.3 (2)
C5—C4—H4	120.4	C21—C22—H22	119.3
N1—C5—C4	123.1 (2)	C23—C22—H22	119.3

N1—C5—H5	118.5	C22—C23—C24	117.94 (19)
C4—C5—H5	118.5	C22—C23—C26	120.9 (2)
N2—C6—C7	122.9 (2)	C24—C23—C26	121.2 (2)
N2—C6—H6	118.5	C25—C24—C23	120.9 (2)
C7—C6—H6	118.5	C25—C24—H24	119.5
C8—C7—C6	119.0 (2)	C23—C24—H24	119.5
C8—C7—H7	120.5	C20—C25—C24	120.8 (2)
C6—C7—H7	120.5	C20—C25—H25	119.6
C7—C8—C9	119.1 (2)	C24—C25—H25	119.6
C7—C8—H8	120.5	C23—C26—H26A	109.5
C9—C8—H8	120.5	C23—C26—H26B	109.5
C8—C9—C10	118.7 (2)	H26A—C26—H26B	109.5
C8—C9—H9	120.6	C23—C26—H26C	109.5
C10—C9—H9	120.6	H26A—C26—H26C	109.5
N2—C10—C9	122.7 (2)	H26B—C26—H26C	109.5
N2—C10—H10	118.7	C5—N1—C1	117.51 (18)
C9—C10—H10	118.7	C5—N1—Ni1	120.29 (14)
O1—C11—O2	119.64 (18)	C1—N1—Ni1	122.19 (14)
O1—C11—C12	120.77 (18)	C10—N2—C6	117.56 (17)
O2—C11—C12	119.58 (17)	C10—N2—Ni1	125.46 (14)
C17—C12—C13	118.57 (19)	C6—N2—Ni1	116.87 (14)
C17—C12—C11	120.52 (19)	O3—Ni1—O1W	94.41 (6)
C13—C12—C11	120.87 (18)	O3—Ni1—N1	86.71 (6)
C14—C13—C12	120.61 (19)	O1W—Ni1—N1	89.53 (6)
C14—C13—H13	119.7	O3—Ni1—N2	89.22 (6)
C12—C13—H13	119.7	O1W—Ni1—N2	92.99 (6)
C13—C14—C15	121.1 (2)	N1—Ni1—N2	175.36 (7)
C13—C14—H14	119.4	O3—Ni1—O2	165.26 (7)
C15—C14—H14	119.4	O1W—Ni1—O2	99.83 (8)
C14—C15—C16	118.13 (19)	N1—Ni1—O2	89.57 (6)
C14—C15—C18	120.9 (2)	N2—Ni1—O2	93.83 (6)
C16—C15—C18	121.0 (2)	O3—Ni1—O1	104.00 (6)
C17—C16—C15	121.1 (2)	O1W—Ni1—O1	161.59 (5)
C17—C16—H16	119.5	N1—Ni1—O1	91.67 (6)
C15—C16—H16	119.5	N2—Ni1—O1	87.17 (6)
C16—C17—C12	120.4 (2)	O2—Ni1—O1	61.82 (7)
C16—C17—H17	119.8	C11—O1—Ni1	87.92 (12)
C12—C17—H17	119.8	C11—O2—Ni1	90.59 (12)
C15—C18—H18A	109.5	C19—O3—Ni1	123.76 (14)
C15—C18—H18B	109.5	Ni1—O1W—H2W	104.8 (19)
H18A—C18—H18B	109.5	Ni1—O1W—H1W	117.0 (18)
C15—C18—H18C	109.5	H2W—O1W—H1W	105.6 (15)
H18A—C18—H18C	109.5		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H2*W*···O4	0.82 (1)	1.83 (1)	2.587 (2)	152 (2)

O1*W*—H1*W*···O1^{i}	0.81 (1)	1.96 (1)	2.739 (2)	162 (2)

Symmetry code: (i) *x*, *y*+1, *z*.