Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

trans-Diaquabis(4-fluorobenzoato-κO)-bis(nicotinamide-κN^1)nickel(II)

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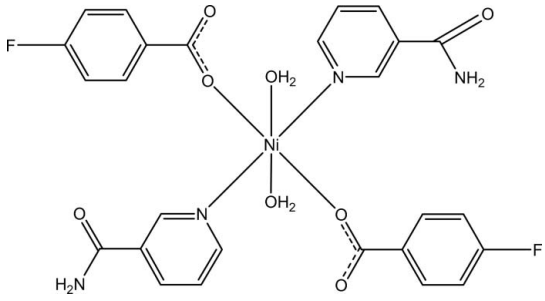
Received 21 October 2011; accepted 26 October 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.077; data-to-parameter ratio = 15.9.

In the mononuclear Ni^{II} title complex, $[Ni(C_7H_4FO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$, the Ni^{II} atom, located on an inversion center, is coordinated by two nicotinamide and two 4-fluorobenzoate ligands and two water molecules in a distorted N_2O_4 octahedral geometry. The dihedral angle between the carboxylate group and the adjacent benzene ring is 8.95 (8)°, while the pyridine ring and the benzene ring are oriented at a dihedral angle of 75.01 (7)°. The water molecule links the adjacent carboxylate O atom *via* an intramolecular O—H···O hydrogen bond. In the crystal, O—H···O, N—H···O, C—H···O and C—H···F hydrogen bonds link the molecules into a three-dimensional network. π–π stacking between parallel pyridine rings [centroid–centroid distance = 3.7287 (11) Å] is also observed.

Related literature

For literature on niacin, see: Krishnamachari (1974). For information on the nicotinic acid derivative *N*,*N*-diethylnicotinamide, see: Bigoli *et al.* (1972). For related structures, see: Hökelek *et al.* (1996, 2009*a*,*b*); Hökelek & Necefoğlu (1998, 2007); Necefoğlu *et al.* (2011). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Ni(C_7H_4FO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$
M_r = 617.18
Monoclinic, $P2_1/c$
a = 12.2001 (5) Å
b = 8.8473 (4) Å
c = 17.1341 (5) Å
β = 136.080 (2)°
V = 1282.86 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.83 mm^{-1}
T = 100 K
0.29 × 0.22 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.803, T_{max} = 0.861
11926 measured reflections
3220 independent reflections
2874 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.077
S = 1.04
3220 reflections
203 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—O1	2.0500 (9)	Ni1—N1	2.1033 (13)
Ni1—O4	2.0872 (10)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H21···O3^{i}	0.84 (3)	2.15 (3)	2.8363 (19)	139 (2)
N2—H22···O4^{ii}	0.86 (3)	2.28 (3)	2.955 (2)	135 (2)
O4—H41···O3^{iii}	0.841 (18)	1.94 (2)	2.7654 (16)	166 (3)
O4—H42···O2	0.88 (3)	1.70 (2)	2.5663 (14)	168 (4)
C6—H6···O4^{iv}	0.93	2.52	3.402 (3)	159
C8—H8···F1^{v}	0.93	2.53	3.1358 (18)	123
C9—H9···F1^{v}	0.93	2.55	3.129 (2)	121
C10—H10···O2^{vi}	0.93	2.57	3.4060 (19)	150

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

The authors are indebted to Anadolu University and the Medicinal Plants and Medicine Research Centre of Anadolu University, Eskişehir, Turkey, for the use of the X-ray diffractometer. This work was supported financially by the Scientific and Technological Research Council of Turkey (grant No. 106 T472).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5359).

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supporting information

Acta Cryst. (2011). E**67**, m1638–m1639 [doi:10.1107/S1600536811044771]

trans-Diaquabis(4-fluorobenzoato-κO)bis(nicotinamide-κN^1)nickel(II)

Hacali Necefoğlu, Vijdan Öztürk, Füreya Elif Özbek, Vedat Adıgüzel and Tuncer Hökelek

S1. Comment

As a part of our ongoing investigations of transition metal complexes of nicotinamide (NA), one form of niacin (Krishnamachari, 1974), and/or the nicotinic acid derivative *N*,*N*-diethylnicotinamide (DENA), an important respiratory stimulant (Bigoli *et al.*, 1972), the title compound was synthesized and its crystal structure is reported herein.

The asymmetric unit of the title mononuclear Ni^{II} complex, (Fig. 1), contains one-half molecule, the Ni^{II} atom being located on an inversion center. It consists of two nicotinamide (NA), two 4-fluorobenzoate (PFB) ligands and two coordinated water molecules, all ligands coordinating in a monodentate manner. The crystal structures of similar omplexes of Cu^{II}, Co^{II}, Ni^{II}, Mn^{II} and Zn^{II} ions, $[Cu(C_7H_5O_2)_2(C_{10}H_{14}N_2O)_2]$ (Hökelek *et al.*, 1996), $[Co(C_6H_6N_2O)_2(C_7H_4NO_4)_2(H_2O)_2]$ (Hökelek & Necefouglu, 1998), $[Co(C_9H_9O_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$ (Necefoğlu *et al.*, 2011), $[Ni(C_7H_4ClO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$ (Hökelek *et al.*, 2009*a*), $[Mn(C_9H_{10}NO_2)_2(H_2O)_4].2H_2O$ (Hökelek & Necefoğlu, 2007) and $[Zn(C_7H_4BrO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$ (Hökelek *et al.*, 2009*b*) have also been reported. In the copper(II) complex mentioned above the two benzoate ions coordinate to the Cu^{II} atom as bidentate ligands, while in the other structures all the ligands coordinate in a monodentate manner.

In the title complex, the four symmetry related O atoms (O1, O1′, O4 and O4′) in the equatorial plane around the Ni^{II} ion form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two N atoms of the NA ligands (N1 and N1′) in the axial positions. The near equalities of the C1—O1 [1.2695 (18) Å] and C1—O2 [1.2560 (16) Å] bonds in the carboxylate groups indicate delocalized bonding arrangements, rather than localized single and double bonds. The Ni—O bond lengths are 2.0500 (9) Å (for benzoate oxygen) and 2.0872 (10) Å (for water oxygen), and the Ni—N bond length is 2.1033 (13) Å, close to standard values (Allen *et al.*, 1987). The intramolecular O—H···O hydrogen bonds (Table 1) link the water molecules to the carboxylate groups. The Ni atom is displaced out of the mean-plane of the carboxylate group (O1/C1/O2) by 0.5609 (1) Å. The dihedral angle between the planar carboxylate group and the adjacent benzene ring A (C2—C7) is 8.95 (8)°. The benzene A (C2—C7) and the pyridine B (N1/C8—C12) rings are oriented at a dihedral angle of A/B = 75.01 (7)°.

In the crystal, intermolecular O—H···O, N—H···O, C—H···O and C—H···F hydrogen bonds (Table 1) link the molecules into a three-dimensional network. There also exists a π–π contact between the pyridine rings, Cg2—Cg2^{i}, may further stabilize the structure [centroid-centroid distance = 3.729 (1) Å; symmetry code: (i) 2 - x, -y, 1 - z; Cg2 is the centroid of the ring B (N1/C8—C12)].

S2. Experimental

The title compound was prepared by the reaction of $NiSO_4.6H_2O$ (1.31 g, 5 mmol) in H_2O (25 ml) and NA (1.22 g, 10 mmol) in H_2O (25 ml) with sodium 4-fluorobenzoate (1.62 g, 10 mmol) in H_2O (100 ml) at room temperature. The mixture was filtered and set aside to crystallize at ambient temperature for two weeks, giving blue single crystals.

S3. Refinement

Atoms H41 and H42 (for water molecules) and H21 and H22 (for NH_2 groups) were located in a difference Fourier map and were freely refined. The C-bound H-atoms were positioned geometrically with C—H = 0.93 Å, for aromatic H-atoms, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

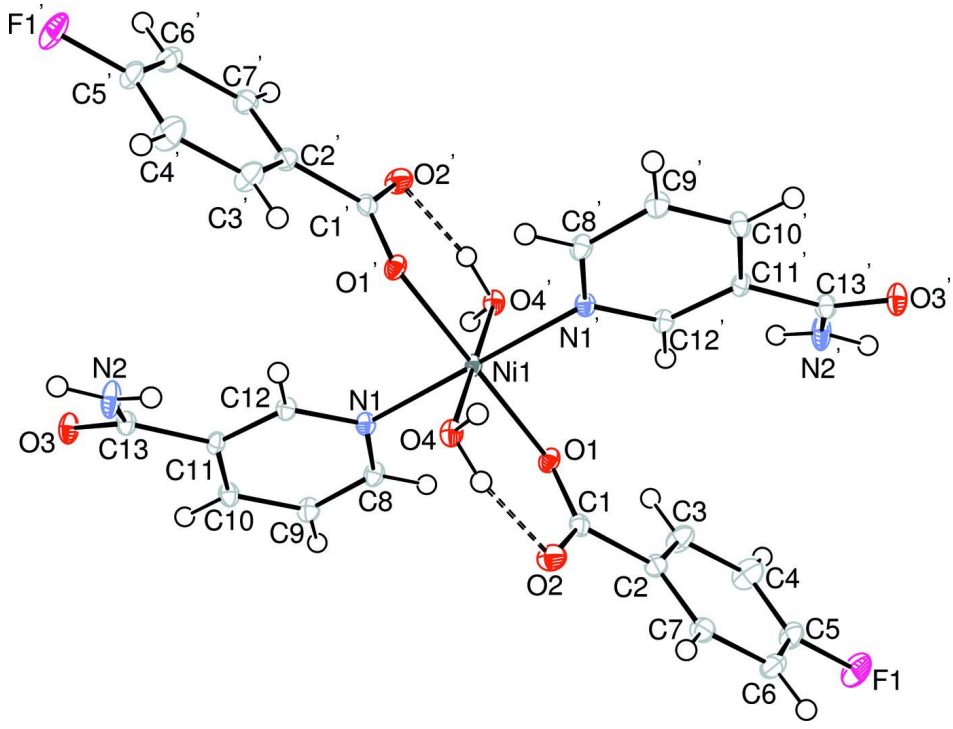

Figure 1

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry code (′): -x, 1-y, 1-z].

trans-Diaquabis(4-fluorobenzoato-κO)bis(nicotinamide- κN^1)nickel(II)

Crystal data

$[Ni(C_7H_4FO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$
M_r = 617.18
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 12.2001 (5) Å
b = 8.8473 (4) Å
c = 17.1341 (5) Å
β = 136.080 (2)°
V = 1282.86 (10) Å^3
Z = 2
$F(000)$ = 636
D_x = 1.598 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6642 reflections
θ = 2.4–28.5°
μ = 0.83 mm^{-1}
T = 100 K
Block, blue
0.29 × 0.22 × 0.18 mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.803, T_{max} = 0.861
11926 measured reflections
3220 independent reflections
2874 reflections with $I > 2\sigma(I)$

R_{int} = 0.028
θ_{max} = 28.5°, θ_{min} = 2.4°
h = −16→16
k = −11→11
l = −22→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.077
S = 1.04
3220 reflections
203 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.038P)^2 + 0.689P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.5000	0.5000	0.00935 (8)
O1	0.18950 (11)	0.45525 (13)	0.66805 (8)	0.0129 (2)
O2	0.35932 (12)	0.35155 (14)	0.66999 (8)	0.0182 (2)
O3	0.04376 (12)	1.15787 (12)	0.34180 (8)	0.0152 (2)
O4	0.11757 (12)	0.41708 (13)	0.46215 (8)	0.0127 (2)
H41	0.088 (2)	0.333 (2)	0.4293 (16)	0.020 (5)*
H42	0.209 (3)	0.398 (3)	0.532 (2)	0.049 (7)*
N1	0.08897 (13)	0.71649 (14)	0.52032 (9)	0.0114 (2)
N2	−0.00057 (17)	0.93579 (17)	0.26006 (11)	0.0180 (3)
H21	0.003 (2)	0.841 (3)	0.2615 (17)	0.030 (6)*
H22	−0.033 (3)	0.984 (3)	0.203 (2)	0.037 (6)*
F1	0.65268 (11)	0.13200 (13)	1.13785 (7)	0.0274 (2)
C1	0.31188 (15)	0.37925 (17)	0.71362 (11)	0.0124 (3)
C2	0.40420 (15)	0.31422 (18)	0.82813 (11)	0.0132 (3)
C3	0.36738 (18)	0.3548 (2)	0.88572 (12)	0.0192 (3)
H3	0.2866	0.4236	0.8538	0.023*
C4	0.45092 (19)	0.2929 (2)	0.99065 (12)	0.0229 (4)
H4	0.4270	0.3190	1.0296	0.027*
C5	0.56940 (17)	0.1923 (2)	1.03506 (11)	0.0185 (3)
C6	0.60852 (17)	0.14784 (19)	0.98051 (12)	0.0176 (3)
H6	0.6885	0.0779	1.0127	0.021*

C7	0.52424 (16)	0.21111 (18)	0.87575 (11)	0.0152 (3)
H7	0.5487	0.1840	0.8372	0.018*
C8	0.18734 (16)	0.78640 (18)	0.62049 (11)	0.0130 (3)
H8	0.2178	0.7358	0.6813	0.016*
C9	0.24541 (16)	0.93048 (18)	0.63733 (11)	0.0141 (3)
H9	0.3144	0.9750	0.7082	0.017*
C10	0.19927 (17)	1.00725 (17)	0.54715 (12)	0.0130 (3)
H10	0.2353	1.1048	0.5560	0.016*
C11	0.09784 (15)	0.93567 (17)	0.44284 (11)	0.0107 (3)
C12	0.04647 (15)	0.79094 (17)	0.43349 (11)	0.0112 (3)
H12	−0.0205	0.7430	0.3639	0.013*
C13	0.04432 (16)	1.01818 (17)	0.34384 (11)	0.0121 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01259 (13)	0.00808 (15)	0.00725 (12)	−0.00057 (10)	0.00710 (10)	0.00028 (9)
O1	0.0143 (4)	0.0119 (5)	0.0089 (4)	0.0004 (4)	0.0072 (4)	0.0005 (4)
O2	0.0158 (5)	0.0271 (7)	0.0124 (4)	0.0011 (5)	0.0104 (4)	0.0016 (5)
O3	0.0245 (5)	0.0088 (5)	0.0148 (4)	−0.0002 (4)	0.0149 (4)	0.0003 (4)
O4	0.0166 (5)	0.0115 (6)	0.0104 (4)	−0.0011 (4)	0.0098 (4)	−0.0014 (4)
N1	0.0136 (5)	0.0107 (6)	0.0113 (5)	−0.0001 (5)	0.0094 (4)	0.0003 (5)
N2	0.0330 (7)	0.0096 (7)	0.0146 (6)	−0.0006 (6)	0.0183 (6)	0.0000 (5)
F1	0.0278 (5)	0.0348 (6)	0.0115 (4)	0.0072 (5)	0.0114 (4)	0.0094 (4)
C1	0.0127 (6)	0.0111 (7)	0.0097 (5)	−0.0039 (6)	0.0068 (5)	−0.0015 (5)
C2	0.0127 (6)	0.0146 (8)	0.0098 (5)	−0.0017 (6)	0.0073 (5)	−0.0007 (5)
C3	0.0187 (7)	0.0240 (9)	0.0143 (6)	0.0063 (7)	0.0117 (6)	0.0035 (6)
C4	0.0254 (7)	0.0318 (10)	0.0152 (6)	0.0062 (8)	0.0159 (6)	0.0027 (7)
C5	0.0176 (6)	0.0214 (9)	0.0092 (6)	0.0001 (7)	0.0072 (5)	0.0030 (6)
C6	0.0143 (6)	0.0181 (8)	0.0147 (6)	0.0036 (6)	0.0086 (5)	0.0032 (6)
C7	0.0146 (6)	0.0169 (8)	0.0135 (6)	−0.0008 (6)	0.0100 (5)	−0.0004 (6)
C8	0.0154 (6)	0.0130 (8)	0.0103 (5)	0.0009 (6)	0.0091 (5)	0.0007 (5)
C9	0.0164 (6)	0.0140 (8)	0.0103 (5)	−0.0015 (6)	0.0091 (5)	−0.0018 (6)
C10	0.0163 (6)	0.0097 (7)	0.0139 (6)	−0.0016 (6)	0.0112 (6)	−0.0011 (5)
C11	0.0130 (6)	0.0110 (7)	0.0105 (5)	0.0021 (6)	0.0092 (5)	0.0023 (5)
C12	0.0132 (6)	0.0112 (7)	0.0097 (5)	0.0001 (6)	0.0085 (5)	−0.0004 (5)
C13	0.0146 (6)	0.0122 (7)	0.0114 (6)	0.0001 (6)	0.0100 (5)	0.0005 (5)

Geometric parameters (Å, º)

Ni1—O1	2.0500 (9)	C2—C7	1.386 (2)
Ni1—O1^{i}	2.0500 (9)	C3—C4	1.390 (2)
Ni1—O4	2.0872 (10)	C3—H3	0.9300
Ni1—O4^{i}	2.0872 (10)	C4—H4	0.9300
Ni1—N1	2.1033 (13)	C5—C4	1.369 (2)
Ni1—N1^{i}	2.1033 (13)	C6—C5	1.378 (2)
O1—C1	1.2695 (18)	C6—C7	1.3906 (19)
O2—C1	1.2560 (16)	C6—H6	0.9300

O3—C13	1.2363 (18)	C7—H7	0.9300
O4—H41	0.84 (2)	C8—C9	1.384 (2)
O4—H42	0.88 (3)	C8—H8	0.9300
N1—C8	1.3421 (17)	C9—C10	1.3830 (19)
N1—C12	1.3435 (17)	C9—H9	0.9300
N2—C13	1.3264 (19)	C10—C11	1.3930 (19)
N2—H21	0.84 (2)	C10—H10	0.9300
N2—H22	0.86 (2)	C12—C11	1.383 (2)
F1—C5	1.3570 (16)	C12—H12	0.9300
C1—C2	1.5051 (18)	C13—C11	1.4970 (18)
C2—C3	1.3939 (19)		

O1^{i}—Ni1—O1	180.0	C4—C3—C2	120.28 (14)
O1—Ni1—O4	92.09 (4)	C4—C3—H3	119.9
O1^{i}—Ni1—O4	87.91 (4)	C3—C4—H4	120.9
O1—Ni1—O4^{i}	87.91 (4)	C5—C4—C3	118.16 (13)
O1^{i}—Ni1—O4^{i}	92.09 (4)	C5—C4—H4	120.9
O1—Ni1—N1	91.03 (4)	F1—C5—C4	118.72 (13)
O1^{i}—Ni1—N1	88.97 (4)	F1—C5—C6	117.82 (14)
O1—Ni1—N1^{i}	88.97 (4)	C4—C5—C6	123.46 (13)
O1^{i}—Ni1—N1^{i}	91.03 (4)	C5—C6—C7	117.73 (14)
O4—Ni1—O4^{i}	180.00 (5)	C5—C6—H6	121.1
O4—Ni1—N1	89.05 (4)	C7—C6—H6	121.1
O4^{i}—Ni1—N1	90.95 (4)	C2—C7—C6	120.67 (13)
O4—Ni1—N1^{i}	90.95 (4)	C2—C7—H7	119.7
O4^{i}—Ni1—N1^{i}	89.05 (4)	C6—C7—H7	119.7
N1^{i}—Ni1—N1	180.00 (8)	N1—C8—C9	122.88 (13)
C1—O1—Ni1	127.09 (9)	N1—C8—H8	118.6
Ni1—O4—H41	117.0 (13)	C9—C8—H8	118.6
Ni1—O4—H42	97.2 (15)	C8—C9—H9	120.5
H41—O4—H42	105 (2)	C10—C9—C8	118.96 (13)
C8—N1—Ni1	120.72 (9)	C10—C9—H9	120.5
C8—N1—C12	117.81 (13)	C9—C10—C11	118.73 (14)
C12—N1—Ni1	121.44 (9)	C9—C10—H10	120.6
C13—N2—H21	123.2 (14)	C11—C10—H10	120.6
C13—N2—H22	116.9 (15)	C10—C11—C13	119.43 (13)
H21—N2—H22	120 (2)	C12—C11—C10	118.63 (12)
O1—C1—C2	116.65 (12)	C12—C11—C13	121.92 (12)
O2—C1—O1	125.40 (12)	N1—C12—C11	122.98 (12)
O2—C1—C2	117.93 (13)	N1—C12—H12	118.5
C3—C2—C1	120.28 (13)	C11—C12—H12	118.5
C7—C2—C1	120.01 (12)	O3—C13—N2	121.96 (13)
C7—C2—C3	119.70 (13)	O3—C13—C11	120.56 (12)
C2—C3—H3	119.9	N2—C13—C11	117.48 (14)

O4—Ni1—O1—C1	−10.42 (12)	O2—C1—C2—C7	−8.4 (2)
O4^{i}—Ni1—O1—C1	169.58 (12)	C1—C2—C3—C4	178.94 (15)
N1—Ni1—O1—C1	−99.50 (12)	C7—C2—C3—C4	0.3 (2)

N1^{i}—Ni1—O1—C1	80.50 (12)	C1—C2—C7—C6	−178.74 (14)
O1—Ni1—N1—C8	−24.63 (11)	C3—C2—C7—C6	−0.1 (2)
O1^{i}—Ni1—N1—C8	155.37 (11)	C2—C3—C4—C5	0.2 (3)
O1—Ni1—N1—C12	157.13 (10)	F1—C5—C4—C3	179.47 (15)
O1^{i}—Ni1—N1—C12	−22.87 (10)	C6—C5—C4—C3	−1.0 (3)
O4—Ni1—N1—C8	−116.70 (11)	C7—C6—C5—F1	−179.28 (14)
O4^{i}—Ni1—N1—C8	63.30 (11)	C7—C6—C5—C4	1.2 (3)
O4—Ni1—N1—C12	65.06 (10)	C5—C6—C7—C2	−0.6 (2)
O4^{i}—Ni1—N1—C12	−114.94 (10)	N1—C8—C9—C10	0.7 (2)
Ni1—O1—C1—O2	20.1 (2)	C8—C9—C10—C11	−1.0 (2)
Ni1—O1—C1—C2	−158.24 (10)	C9—C10—C11—C12	0.4 (2)
Ni1—N1—C8—C9	−178.10 (10)	C9—C10—C11—C13	178.87 (13)
C12—N1—C8—C9	0.2 (2)	N1—C12—C11—C10	0.5 (2)
Ni1—N1—C12—C11	177.43 (10)	N1—C12—C11—C13	−177.86 (12)
C8—N1—C12—C11	−0.86 (19)	O3—C13—C11—C10	−23.7 (2)
O1—C1—C2—C3	−8.6 (2)	O3—C13—C11—C12	154.64 (13)
O1—C1—C2—C7	170.00 (14)	N2—C13—C11—C10	155.73 (14)
O2—C1—C2—C3	172.92 (14)	N2—C13—C11—C12	−25.9 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H21···O3^{ii}	0.84 (3)	2.15 (3)	2.8363 (19)	139 (2)
N2—H22···O4^{iii}	0.86 (3)	2.28 (3)	2.955 (2)	135 (2)
O4—H41···O3^{iv}	0.841 (18)	1.94 (2)	2.7654 (16)	166 (3)
O4—H42···O2	0.88 (3)	1.70 (2)	2.5663 (14)	168 (4)
C6—H6···O4^{v}	0.93	2.52	3.402 (3)	159
C8—H8···F1^{vi}	0.93	2.53	3.1358 (18)	123
C9—H9···F1^{vi}	0.93	2.55	3.129 (2)	121
C10—H10···O2^{vii}	0.93	2.57	3.4060 (19)	150

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