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

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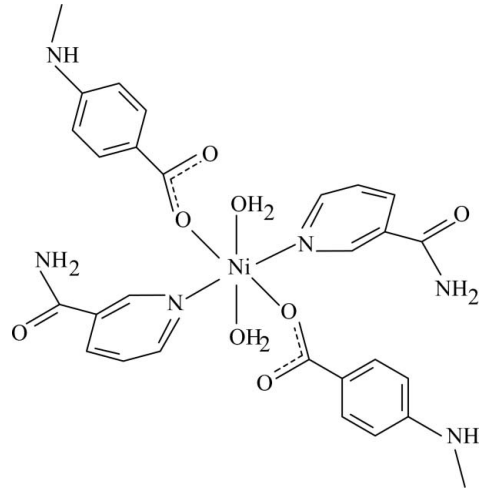
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.085; data-to-parameter ratio = 16.8.

The title Ni^{II} complex, $[Ni(C_8H_8NO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$, is centrosymmetric with the Ni atom on an inversion center. The molecule contains two 4-methylaminobenzoate (MAB) and two nicotinamide (NA) ligands and two coordinated water molecules, all ligands being monodentate. The four O atoms in the equatorial plane around the Ni atom form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two N atoms of the NA ligands in the axial positions. The dihedral angle between the carboxylate group and the adjacent benzene ring is 2.09 (14)°, while the pyridine and benzene rings are oriented at a dihedral angle of 66.15 (4)°. In the crystal structure, intermolecular O—H···O and N—H···O hydrogen bonds link the molecules into a three-dimensional network.

Related literature

For general background to transition metal complexes with biochemically active ligands, see: Antolini *et al.* (1982); Bigoli *et al.* (1972); Nadzhafov *et al.* (1981); Shnulin *et al.* (1981); Krishnamachari (1974). For related structures, see: Hökelek *et al.* (1995, 1997, 2007, 2008); Hökelek & Necefoğlu (1996, 1997, 2007).



Experimental

Crystal data

$[Ni(C_8H_8NO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$
M_r = 639.31
Monoclinic, $P2_1/n$
a = 10.9331 (6) Å
b = 9.8467 (5) Å
c = 14.1992 (8) Å
β = 107.454 (1)°
V = 1458.23 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 100 K
0.47 × 0.32 × 0.31 mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.755, T_{max} = 0.796
13201 measured reflections
3635 independent reflections
2954 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.085
S = 1.09
3635 reflections
217 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—O1	2.0362 (9)	Ni1—N1	2.0903 (13)
Ni1—O4	2.0800 (11)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H21···O2^{i}	0.92 (2)	2.01 (2)	2.9150 (18)	167.9 (18)
N3—H31···O4^{ii}	0.84 (2)	2.44 (2)	3.162 (2)	144.6 (19)
O4—H41···O3^{iii}	0.877 (15)	1.808 (15)	2.6849 (16)	179 (2)
O4—H42···O2^{iv}	0.89 (2)	1.80 (2)	2.6464 (15)	156 (2)

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

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2516).

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supporting information

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

Tuncer Hökelek, Hakan Dal, Barış Tercan, Özgür Aybirdi and Hacali Necefoğlu

S1. Comment

Transition metal complexes with biochemically active ligands frequently show interesting physical and/or chemical properties, as a result they may find applications in biological systems (Antolini *et al.*, 1982). The structural functions and coordination relationships of the arylcarboxylate ion in transition metal complexes of benzoic acid derivatives change depending on the nature and position of the substituent groups on the benzene ring, the nature of the additional ligand molecule or solvent, and the medium of the synthesis (Nadzhafov *et al.*, 1981; Shnulin *et al.*, 1981). Nicotinamide (NA) is one form of niacin and a deficiency of this vitamin leads to loss of copper from the body, known as pellagra disease. Victims of pellagra show unusually high serum and urinary copper levels (Krishnamachari, 1974). On the other hand, the nicotinic acid derivative *N*,*N*-diethylnicotinamide (DENA) is an important respiratory stimulant (Bigoli *et al.*, 1972).

The structure determination of the title compound, (I), a nickel complex with two 4-methylaminobenzoate (MAB), two nicotinamide (NA) ligands and two water molecules, was undertaken in order to determine the properties of the ligands and also to compare the results obtained with those reported previously.

Compound (I) is a monomeric complex, with the Ni atom on a centre of symmetry. It contains two MAB, two NA ligands and two water molecules (Fig. 1). All ligands are monodentate. The four O atoms (O1, O4, and the symmetry-related atoms, O1′, O4′) in the equatorial plane around the Ni atom 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, N1′) in the axial positions (Fig. 1).

The near equality of the C1—O1 [1.2746 (18) Å] and C1—O2 [1.2675 (17) Å] bonds in the carboxylate group indicates a delocalized bonding arrangement, rather than localized single and double bonds, and may be compared with the corresponding distances: 1.256 (6) and 1.245 (6) Å in $[Mn(DENA)_2(C_7H_4ClO_2)_2(H_2O)_2]$, (II) (Hökelek *et al.*, 2008), 1.265 (6) and 1.275 (6) Å in $[Mn(C_9H_{10}NO_2)_2(H_2O)_4].2(H_2O)$, (III) (Hökelek & Necefoğlu, 2007), 1.260 (4) and 1.252 (4) Å in $[Zn(DENA)_2(C_7H_4FO_2)_2(H_2O)_2]$,(IV) (Hökelek *et al.*, 2007), 1.259 (9) and 1.273 (9) Å in $Cu_2(DENA)_2(C_6H_5COO)_4$, (V) (Hökelek *et al.*, 1995), 1.279 (4) and 1.246 (4) Å in $[Zn_2(DENA)_2(C_7H_5O_3)_4].2H_2O$, (VI) (Hökelek & Necefoğlu, 1996), 1.251 (6) and 1.254 (7) Å in $[Co(DENA)_2(C_7H_5O_3)_2(H_2O)_2]$, (VII) (Hökelek & Necefoğlu, 1997) and 1.278 (3) and 1.246 (3) Å in $[Cu(DENA)_2(C_7H_4NO_4)_2(H_2O)_2]$, (VIII) (Hökelek *et al.*, 1997). In (I), the average Ni—O bond length is 2.0581 (10) Å and the Ni atom is displaced out of the least-squares plane of the carboxylate group (O1/C1/O2) by -0.395 (1) Å. The dihedral angle between the planar carboxylate group and the benzene ring A (C2—C7) is 2.09 (14)°, while that between rings A and B (N1/C8—C12) is 66.15 (4)°.

In the crystal structure, intermolecular O—H···O and N—H···O hydrogen bonds (Table 1) link the molecules into a three-dimensional network, in which they may be effective in the stabilization of the structure.

S2. Experimental

The title compound was prepared by the reaction of $NiSO_4.6(H_2O)$ (1.31 g, 5 mmol) in H_2O (30 ml) and NA (1.22 g, 10 mmol) in H_2O (20 ml) with sodium 4-methylaminobenzoate (1.51 g, 10 mmol) in H_2O (50 ml). The mixture was filtered and set aside to crystallize at ambient temperature for one week, giving blue single crystals.

S3. Refinement

H atoms of water molecule, NH and NH_2 groups were located in difference Fourier maps and refined isotropically, with restrains of O4—H41 = 0.878 (14) and O4 H42 = 0.897 (16) Å and H41—O4—H42 = 105.4 (18)°. The remaining H atoms were positioned geometrically with C—H = 0.93 and 0.96 Å, for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.5$ for methyl H and $x = 1.2$ for aromatic H atoms.

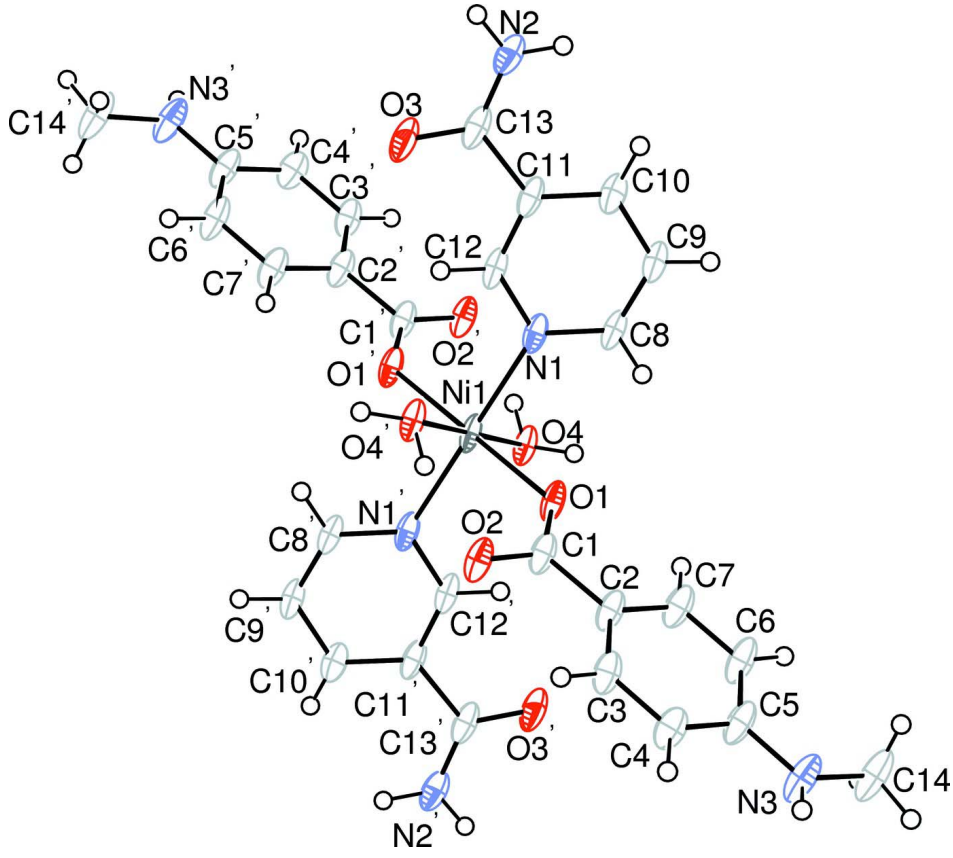

Figure 1

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Primed atoms are generated by the symmetry operator (- *x*, 1-*y*, -*z*).

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Crystal data

$[Ni(C_8H_8NO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$
$M_r = 639.31$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.9331$ (6) Å
$b = 9.8467$ (5) Å
$c = 14.1992$ (8) Å
$\beta = 107.454$ (1)°
$V = 1458.23$ (14) Å^3
$Z = 2$

$F(000) = 668$
$D_x = 1.456$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6218 reflections
$\theta = 2.6$–$28.4°$
$\mu = 0.73$ mm^{-1}
$T = 100$ K
Block, blue
0.47 × 0.32 × 0.31 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)
$T_{min} = 0.755$, $T_{max} = 0.796$
13201 measured reflections
3635 independent reflections
2954 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 28.4°$, $\theta_{min} = 2.1°$
$h = -14 \rightarrow 13$
$k = -12 \rightarrow 13$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.085$
$S = 1.09$
3635 reflections
217 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 0.1097P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Ni1	0.0000	0.5000	0.0000	0.02520 (9)
O1	−0.05431 (9)	0.42926 (11)	0.11617 (7)	0.0298 (2)
O2	−0.20986 (10)	0.28374 (11)	0.03794 (7)	0.0331 (3)
O3	−0.24476 (12)	0.91313 (14)	−0.21749 (8)	0.0441 (3)
O4	0.18759 (10)	0.52817 (12)	0.08904 (8)	0.0295 (2)
H41	0.209 (2)	0.547 (2)	0.1523 (11)	0.055 (6)*
H42	0.212 (2)	0.600 (2)	0.0608 (16)	0.087 (9)*
N1	−0.05647 (11)	0.69514 (13)	0.02746 (8)	0.0269 (3)
N2	−0.23426 (13)	1.10935 (16)	−0.13262 (11)	0.0354 (3)
H21	−0.217 (2)	1.156 (2)	−0.0742 (16)	0.062 (6)*
H22	−0.2690 (18)	1.1511 (18)	−0.1881 (14)	0.039 (5)*

N3	−0.12888 (14)	0.12206 (18)	0.48807 (10)	0.0422 (4)
H31	−0.190 (2)	0.071 (2)	0.4877 (16)	0.061 (7)*
C1	−0.13324 (13)	0.33378 (16)	0.11561 (10)	0.0290 (3)
C2	−0.13399 (13)	0.28004 (16)	0.21324 (10)	0.0291 (3)
C3	−0.21846 (14)	0.17675 (17)	0.22136 (11)	0.0305 (3)
H3	−0.2773	0.1428	0.1646	0.037*
C4	−0.21573 (14)	0.12488 (17)	0.31176 (11)	0.0328 (3)
H4	−0.2723	0.0559	0.3152	0.039*
C5	−0.12885 (14)	0.17437 (18)	0.39904 (11)	0.0335 (4)
C6	−0.04453 (14)	0.27794 (18)	0.39144 (11)	0.0368 (4)
H6	0.0145	0.3121	0.4481	0.044*
C7	−0.04892 (14)	0.32956 (18)	0.29965 (11)	0.0334 (3)
H7	0.0067	0.3994	0.2959	0.040*
C8	−0.04561 (13)	0.74589 (17)	0.11720 (10)	0.0288 (3)
H8	−0.0069	0.6930	0.1723	0.035*
C9	−0.08955 (14)	0.87357 (17)	0.13112 (11)	0.0321 (3)
H9	−0.0814	0.9052	0.1944	0.039*
C10	−0.14588 (14)	0.95401 (18)	0.04957 (11)	0.0315 (3)
H10	−0.1749	1.0409	0.0571	0.038*
C11	−0.15803 (13)	0.90173 (16)	−0.04382 (10)	0.0287 (3)
C12	−0.11315 (13)	0.77289 (17)	−0.05083 (10)	0.0285 (3)
H12	−0.1227	0.7378	−0.1134	0.034*
C13	−0.21654 (14)	0.97680 (18)	−0.13847 (11)	0.0333 (4)
C14	−0.04606 (17)	0.1690 (2)	0.58153 (12)	0.0495 (5)
H14A	−0.0642	0.1195	0.6340	0.074*
H14B	−0.0605	0.2641	0.5888	0.074*
H14C	0.0417	0.1547	0.5841	0.074*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01580 (14)	0.04990 (18)	0.01093 (13)	−0.00137 (10)	0.00555 (10)	−0.00041 (10)
O1	0.0223 (5)	0.0548 (7)	0.0150 (5)	−0.0029 (4)	0.0097 (4)	−0.0004 (4)
O2	0.0224 (5)	0.0601 (7)	0.0174 (5)	−0.0052 (5)	0.0070 (4)	0.0009 (5)
O3	0.0456 (7)	0.0668 (8)	0.0148 (5)	0.0090 (6)	0.0013 (5)	0.0035 (5)
O4	0.0196 (5)	0.0539 (7)	0.0139 (5)	−0.0019 (4)	0.0037 (4)	−0.0018 (4)
N1	0.0163 (5)	0.0507 (7)	0.0146 (6)	−0.0017 (5)	0.0061 (5)	0.0002 (5)
N2	0.0270 (7)	0.0584 (9)	0.0188 (7)	0.0069 (6)	0.0037 (6)	0.0069 (6)
N3	0.0257 (7)	0.0787 (11)	0.0224 (7)	−0.0043 (7)	0.0074 (6)	0.0137 (7)
C1	0.0172 (7)	0.0540 (9)	0.0179 (7)	0.0031 (6)	0.0086 (6)	0.0016 (6)
C2	0.0168 (6)	0.0542 (9)	0.0185 (7)	0.0036 (6)	0.0087 (5)	0.0045 (6)
C3	0.0181 (7)	0.0548 (9)	0.0204 (7)	0.0017 (6)	0.0084 (6)	−0.0003 (6)
C4	0.0203 (7)	0.0547 (10)	0.0267 (8)	0.0006 (6)	0.0119 (6)	0.0055 (7)
C5	0.0190 (7)	0.0630 (10)	0.0206 (7)	0.0058 (6)	0.0092 (6)	0.0100 (7)
C6	0.0200 (7)	0.0717 (11)	0.0175 (7)	−0.0031 (7)	0.0035 (6)	0.0058 (7)
C7	0.0193 (7)	0.0609 (10)	0.0211 (7)	−0.0022 (6)	0.0078 (6)	0.0058 (7)
C8	0.0196 (7)	0.0541 (9)	0.0130 (6)	0.0013 (6)	0.0052 (5)	0.0034 (6)
C9	0.0268 (7)	0.0552 (9)	0.0146 (7)	0.0030 (7)	0.0066 (6)	−0.0005 (6)

C10	0.0226 (7)	0.0537 (9)	0.0188 (7)	0.0038 (6)	0.0072 (6)	0.0012 (6)
C11	0.0151 (6)	0.0558 (9)	0.0148 (7)	0.0000 (6)	0.0038 (5)	0.0027 (6)
C12	0.0172 (6)	0.0556 (9)	0.0128 (6)	−0.0017 (6)	0.0046 (5)	−0.0002 (6)
C13	0.0191 (7)	0.0634 (11)	0.0162 (7)	0.0035 (6)	0.0037 (6)	0.0047 (6)
C14	0.0309 (9)	0.0953 (15)	0.0205 (8)	−0.0025 (9)	0.0053 (7)	0.0164 (9)

Geometric parameters (Å, º)

Ni1—O1	2.0362 (9)	C3—C4	1.373 (2)
Ni1—O1^{i}	2.0362 (9)	C3—H3	0.9300
Ni1—O4	2.0800 (11)	C4—H4	0.9300
Ni1—O4^{i}	2.0800 (11)	C5—N3	1.3652 (19)
Ni1—N1	2.0903 (13)	C5—C4	1.403 (2)
Ni1—N1^{i}	2.0903 (13)	C5—C6	1.400 (2)
O1—C1	1.2746 (18)	C6—C7	1.386 (2)
O2—C1	1.2675 (17)	C6—H6	0.9300
O3—C13	1.2407 (19)	C7—H7	0.9300
O4—H41	0.878 (14)	C8—C9	1.381 (2)
O4—H42	0.897 (16)	C8—H8	0.9300
N1—C8	1.3404 (17)	C9—C10	1.386 (2)
N1—C12	1.3389 (18)	C9—H9	0.9300
N2—C13	1.326 (2)	C10—H10	0.9300
N2—H21	0.92 (2)	C11—C10	1.391 (2)
N2—H22	0.869 (19)	C11—C12	1.375 (2)
N3—C14	1.440 (2)	C11—C13	1.499 (2)
N3—H31	0.83 (2)	C12—H12	0.9300
C2—C1	1.4861 (19)	C14—H14A	0.9600
C2—C7	1.387 (2)	C14—H14B	0.9600
C3—C2	1.402 (2)	C14—H14C	0.9600
O1^{i}—Ni1—O1	180.0	C3—C4—C5	121.02 (15)
O1—Ni1—O4	91.56 (4)	C3—C4—H4	119.5
O1^{i}—Ni1—O4	88.44 (4)	C5—C4—H4	119.5
O1^{i}—Ni1—O4^{i}	91.56 (4)	N3—C5—C4	119.91 (15)
O1—Ni1—O4^{i}	88.44 (4)	N3—C5—C6	121.94 (15)
O1—Ni1—N1	89.38 (4)	C6—C5—C4	118.14 (13)
O1^{i}—Ni1—N1	90.62 (4)	C5—C6—H6	120.0
O1—Ni1—N1^{i}	90.62 (4)	C7—C6—C5	120.10 (14)
O1^{i}—Ni1—N1^{i}	89.38 (4)	C7—C6—H6	120.0
O4—Ni1—O4^{i}	180.00 (7)	C2—C7—H7	119.1
O4—Ni1—N1	93.24 (4)	C6—C7—C2	121.85 (15)
O4^{i}—Ni1—N1	86.76 (4)	C6—C7—H7	119.1
O4—Ni1—N1^{i}	86.76 (4)	N1—C8—C9	122.69 (13)
O4^{i}—Ni1—N1^{i}	93.24 (4)	N1—C8—H8	118.7
N1^{i}—Ni1—N1	180.00 (6)	C9—C8—H8	118.7
C1—O1—Ni1	127.49 (9)	C8—C9—C10	119.16 (14)
Ni1—O4—H41	123.9 (14)	C8—C9—H9	120.4
Ni1—O4—H42	102.0 (16)	C10—C9—H9	120.4

H41—O4—H42	105.4 (18)	C9—C10—C11	118.46 (15)
C8—N1—Ni1	124.97 (10)	C9—C10—H10	120.8
C12—N1—Ni1	117.37 (9)	C11—C10—H10	120.8
C12—N1—C8	117.58 (13)	C10—C11—C13	124.42 (15)
C13—N2—H21	123.9 (13)	C12—C11—C10	118.45 (13)
C13—N2—H22	116.2 (12)	C12—C11—C13	117.12 (13)
H21—N2—H22	119.8 (18)	N1—C12—C11	123.64 (13)
C5—N3—C14	123.89 (16)	N1—C12—H12	118.2
C5—N3—H31	116.4 (15)	C11—C12—H12	118.2
C14—N3—H31	118.7 (15)	O3—C13—N2	123.55 (15)
O1—C1—C2	116.74 (13)	O3—C13—C11	119.03 (15)
O2—C1—O1	124.17 (13)	N2—C13—C11	117.41 (14)
O2—C1—C2	119.08 (13)	N3—C14—H14A	109.5
C3—C2—C1	121.55 (13)	N3—C14—H14B	109.5
C7—C2—C1	120.67 (13)	N3—C14—H14C	109.5
C7—C2—C3	117.77 (13)	H14A—C14—H14B	109.5
C2—C3—H3	119.4	H14A—C14—H14C	109.5
C4—C3—C2	121.11 (14)	H14B—C14—H14C	109.5
C4—C3—H3	119.4		

O4—Ni1—O1—C1	−142.35 (12)	C1—C2—C7—C6	−177.70 (14)
O4^{i}—Ni1—O1—C1	37.65 (12)	C3—C2—C7—C6	1.3 (2)
N1^{i}—Ni1—O1—C1	−55.58 (12)	C4—C3—C2—C1	177.98 (14)
N1—Ni1—O1—C1	124.42 (12)	C4—C3—C2—C7	−1.0 (2)
O1^{i}—Ni1—N1—C8	−145.11 (11)	C2—C3—C4—C5	0.5 (2)
O1—Ni1—N1—C8	34.89 (11)	C4—C5—N3—C14	−178.12 (16)
O1^{i}—Ni1—N1—C12	38.14 (10)	C6—C5—N3—C14	1.4 (3)
O1—Ni1—N1—C12	−141.86 (10)	N3—C5—C4—C3	179.35 (15)
O4—Ni1—N1—C8	−56.63 (11)	N3—C5—C6—C7	−179.07 (16)
O4^{i}—Ni1—N1—C8	123.37 (11)	C4—C5—C6—C7	0.5 (2)
O4—Ni1—N1—C12	126.62 (10)	C6—C5—C4—C3	−0.2 (2)
O4^{i}—Ni1—N1—C12	−53.38 (10)	C5—C6—C7—C2	−1.1 (3)
Ni1—O1—C1—O2	−14.1 (2)	N1—C8—C9—C10	−0.8 (2)
Ni1—O1—C1—C2	166.19 (9)	C8—C9—C10—C11	1.1 (2)
Ni1—N1—C8—C9	−177.10 (11)	C12—C11—C10—C9	−0.2 (2)
C12—N1—C8—C9	−0.4 (2)	C13—C11—C10—C9	−179.89 (14)
Ni1—N1—C12—C11	178.29 (11)	C10—C11—C12—N1	−1.0 (2)
C8—N1—C12—C11	1.3 (2)	C13—C11—C12—N1	178.68 (13)
C3—C2—C1—O1	178.85 (13)	C10—C11—C13—O3	−166.51 (15)
C3—C2—C1—O2	−0.8 (2)	C10—C11—C13—N2	14.0 (2)
C7—C2—C1—O1	−2.2 (2)	C12—C11—C13—O3	13.8 (2)
C7—C2—C1—O2	178.09 (14)	C12—C11—C13—N2	−165.61 (13)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H21···O2^{ii}	0.92 (2)	2.01 (2)	2.9150 (18)	167.9 (18)

N3—H31···O4^{iii}	0.84 (2)	2.44 (2)	3.162 (2)	144.6 (19)
O4—H41···O3^{iv}	0.88 (2)	1.81 (2)	2.6849 (16)	179 (2)
O4—H42···O2^{i}	0.89 (2)	1.80 (2)	2.6464 (15)	156 (2)

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