Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Tuncer Hökelek,[a]* Hakan Dal,[b] Barış Tercan,[c] Erdinç Tenlik[d] and Hacali Necefoğlu[d]

[a]Department of Physics, Hacettepe University, 06800 Beytepe, Ankara, Turkey, [b]Department of Chemistry, Faculty of Science, Anadolu University, 26470 Yenibağlar, Eskişehir, Turkey, [c]Department of Physics, Karabük University, 78050 Karabük, Turkey, and [d]Department of Chemistry, Kafkas University, 36100 Kars, Turkey
Correspondence e-mail: merzifon@hacettepe.edu.tr

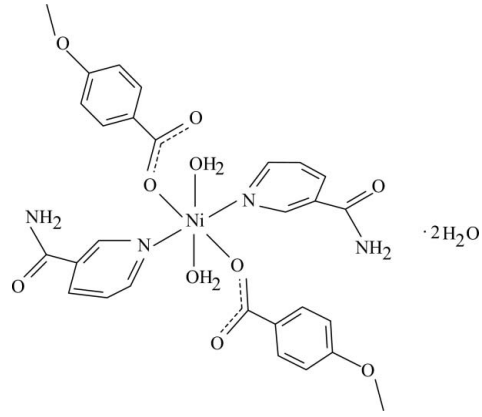
Received 30 June 2010; accepted 1 July 2010

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.026; wR factor = 0.067; data-to-parameter ratio = 16.4.

In the mononuclear title compound, $[Ni(C_8H_7O_3)_2(C_6H_6N_2O)_2(H_2O)_2]\cdot 2H_2O$, the Ni^{II} ion is located on a crystallographic inversion center. The asymmetric unit further contains one 4-methoxybenzoate anion, one nicotinamide (NA) ligand and one coordinated and one uncoordinated water molecule; all ligands are monodentate. The four O atoms 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 pyridine N atoms of the NA ligands in the axial positions. The dihedral angle between the carboxylate group and the attached benzene ring is 7.2 (1)°, while the pyridine and benzene rings are oriented at a dihedral angle of 72.80 (4)°. An intramolecular O—H···O hydrogen bond links the uncoordinated water molecule to one of the carboxylate groups. In the crystal structure, intermolecular O—H···O, N—H···O and C—H···O hydrogen bonds link the molecules into a three-dimensional network.

Related literature

For niacin, see: Krishnamachari (1974). For *N*,*N*-diethylnicotinamide, see: Bigoli *et al.* (1972). For related structures, see: Hökelek *et al.* (1996, 2009*a*,*b*,*c*); Hökelek & Necefoğlu (1998); Necefoğlu *et al.* (2010).



Experimental

Crystal data

$[Ni(C_8H_7O_3)_2(C_6H_6N_2O)_2(H_2O)_2]\cdot 2H_2O$
M_r = 677.28
Triclinic, $P\overline{1}$
a = 8.1279 (2) Å
b = 9.7006 (2) Å
c = 10.0636 (3) Å
α = 101.637 (3)°
β = 91.634 (2)°
γ = 105.137 (3)°
V = 747.42 (4) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.72 mm^{-1}
T = 100 K
0.35 × 0.26 × 0.19 mm

Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.797, T_{max} = 0.871
13749 measured reflections
3740 independent reflections
3454 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.067
S = 1.04
3740 reflections
228 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—O1	2.0569 (9)	Ni1—N1	2.1167 (10)
Ni1—O5	2.0697 (9)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H22···O6^{i}	0.88 (2)	1.96 (2)	2.8306 (16)	170 (2)
O5—H51···O4^{ii}	0.83 (2)	1.88 (2)	2.7074 (14)	171 (2)
O5—H52···O2^{iii}	0.79 (2)	1.95 (2)	2.7040 (14)	159 (2)
O6—H61···O2	0.82 (2)	1.99 (2)	2.8136 (14)	174 (2)
O6—H62···O2^{iv}	0.82 (2)	2.08 (2)	2.8887 (15)	169 (2)
C9—H9···O1^{iii}	0.95	2.35	2.9719 (16)	123
C10—H10···O5^{v}	0.95	2.41	3.2973 (17)	156

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

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 use of the X-ray diffractometer. This work was supported financially by Kafkas University Research Fund (grant No. 2009-FEF-03).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5126).

References

Bigoli, F., Braibanti, A., Pellinghelli, M. A. & Tiripicchio, A. (1972). *Acta Cryst.* B**28**, 962–966.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Hökelek, T., Dal, H., Tercan, B., Özbek, F. E. & Necefoğlu, H. (2009*a*). *Acta Cryst.* E**65**, m466–m467.
Hökelek, T., Dal, H., Tercan, B., Özbek, F. E. & Necefoğlu, H. (2009*b*). *Acta Cryst.* E**65**, m513–m514.
Hökelek, T., Dal, H., Tercan, B., Özbek, F. E. & Necefoğlu, H. (2009*c*). *Acta Cryst.* E**65**, m607–m608.
Hökelek, T., Gündüz, H. & Necefoğlu, H. (1996). *Acta Cryst.* C**52**, 2470–2473.
Hökelek, T. & Necefoğlu, H. (1998). *Acta Cryst.* C**54**, 1242–1244.
Krishnamachari, K. A. V. R. (1974). *Am. J. Clin. Nutr.* **27**, 108–111.
Necefoğlu, H., Çimen, E., Tercan, B., Ermiş, E. & Hökelek, T. (2010). *Acta Cryst.* E**66**, m361–m362.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2010). E**66**, m891–m892 [https://doi.org/10.1107/S1600536810025985]

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

Tuncer Hökelek, Hakan Dal, Barış Tercan, Erdinç Tenlik and Hacali Necefoğlu

S1. Comment

As a part of our ongoing investigation on 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 title compound, (I), is a mononuclear complex, where the Ni^{II} ion is located on a crystallographic inversion center. The asymmetric unit contains one 4-methoxybenzoate (PMOB) anion, one nicotinamide (NA) ligand and one coordinated and one uncoordinated water molecules, all ligands are monodentate (Fig. 1). The crystal structures of some NA and/or DENA complexes of Cu^{II}, Co^{II}, Ni^{II}, Mn^{II} and Zn^{II} ions, $[Cu(C_7H_5O_2)_2(C_{10}H_{14}N_2O)_2]$, (II) (Hökelek *et al.*, 1996), $[Co(C_6H_6N_2O)_2(C_7H_4NO_4)_2(H_2O)_2]$, (III) (Hökelek & Necefoğlu, 1998), $[Ni(C_7H_4ClO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$, (IV) (Hökelek *et al.*, 2009*a*), $[Ni(C_8H_7O_2)_2(C_6H_6N_2O)_2(H_2O)_2]$, (V) (Necefoğlu *et al.*, 2010), $[Mn(C_7H_4ClO_2)_2(C_{10}H_{14}N_2O)_2(H_2O)_2]$, (VI) (Hökelek *et al.*, 2009*b*) and $[Zn(C_7H_4BrO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$, (VII) (Hökelek *et al.*, 2009*c*) have also been reported. In (II), two benzoate ions are coordinated to the Cu atom as bidentate ligands, while in other structures all ligands being monodentate.

The four O atoms (O1, O5, and the symmetry-related atoms, O1′, O5′) 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, N1′) in the axial positions (Fig. 1). The near equality of the C1—O1 [1.2681 (15) Å] and C1—O2 [1.2644 (16) Å] bonds in the carboxylate group indicates a delocalized bonding arrangement, rather than localized single and double bonds. The average Ni—O bond length is 2.0633 (9) Å (Table 1), and the Ni^{II} ion is displaced out of the least-squares plane of the carboxylate group (O1/C1/O2) by 0.7794 (1) Å. The dihedral angle between the planar carboxylate group and the benzene ring A (C2—C7) is 7.2 (1)°, while that between rings A and B (N1/C9—C13) is 72.80 (4)°. An intramolecular O—H···O hydrogen bond (Table 2) links the uncoordinated water molecule to one of the carboxylate groups (Fig. 1).

In the crystal structure, intermolecular O—H···O, N—H···O and C—H···O hydrogen bonds (Table 2) link the molecules into a three-dimensional network.

S2. Experimental

The title compound was prepared by the reaction of $NiSO_4.6H_2O$ (2.63 g, 10 mmol) in H_2O (50 ml) and nicotinamide (2.44 g, 20 mmol) in H_2O (50 ml) with sodium 4-methoybenzoate (3.48 g, 20 mmol) in H_2O (100 ml). The mixture was filtered and set aside to crystallize at ambient temperature for one week, giving blue single crystals.

S3. Refinement

Atoms H21, H22 (for NH_2) and H51, H52, H61, H62 (for H_2O) were located in a difference Fourier map and refined isotropically. The remaining H atoms were positioned geometrically with C—H = 0.95 and 0.98 Å for aromatic and

methyl H atoms 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.

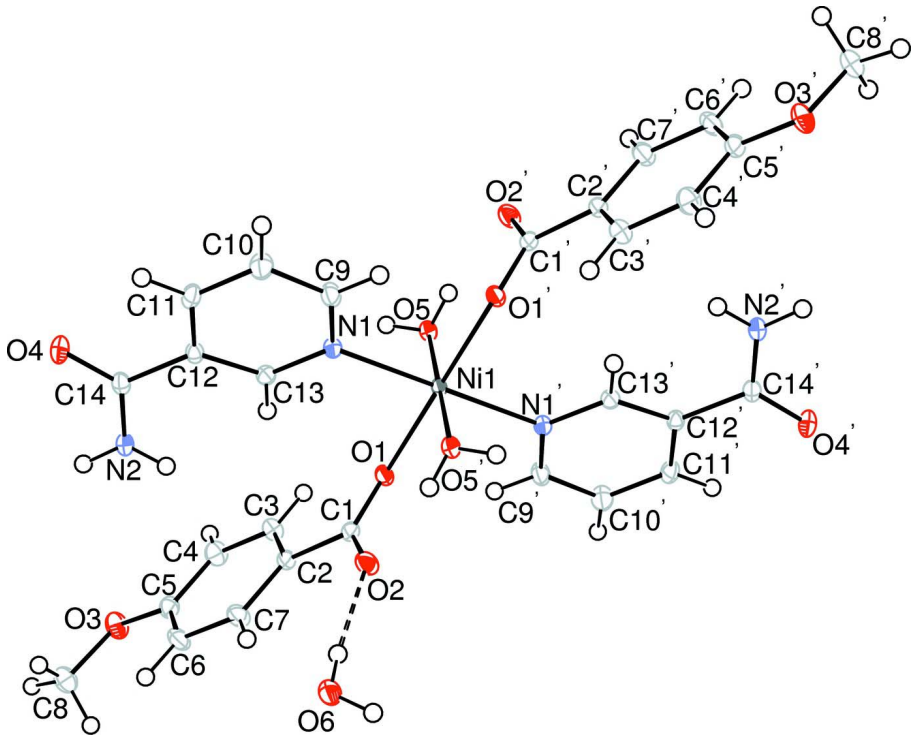


Figure 1

The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Primed atoms are generated by the symmetry operator: (′) 2 - *x*, 1 - *y*, 1 -*z*. Dashed lines indicate the hydrogen-bonding.

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

Crystal data

$[Ni(C_8H_7O_3)_2(C_6H_6N_2O)_2(H_2O)_2]\cdot 2H_2O$
$M_r = 677.28$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.1279$ (2) Å
$b = 9.7006$ (2) Å
$c = 10.0636$ (3) Å
$\alpha = 101.637$ (3)°
$\beta = 91.634$ (2)°
$\gamma = 105.137$ (3)°
$V = 747.42$ (4) Å^3
$Z = 1$
$F(000) = 354$
$D_x = 1.505$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7665 reflections
$\theta = 2.2$–$28.4°$
$\mu = 0.72$ mm^{-1}
$T = 100$ K
Block, blue
0.35 × 0.26 × 0.19 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)
$T_{min} = 0.797$, $T_{max} = 0.871$
13749 measured reflections
3740 independent reflections
3454 reflections with $I > 2\sigma(I)$

R_{int} = 0.024
θ_{max} = 28.4°, θ_{min} = 2.1°
h = −10→10
k = −12→12
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.067
S = 1.04
3740 reflections
228 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
$w = 1/[\sigma^2(F_o^2) + (0.0304P)^2 + 0.3607P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 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}
Ni1	1.0000	0.5000	0.5000	0.01031 (7)
O1	0.84093 (11)	0.34709 (9)	0.34598 (9)	0.01344 (18)
O2	0.97158 (13)	0.37223 (10)	0.15603 (9)	0.0186 (2)
O3	0.51173 (13)	−0.29261 (10)	0.00777 (10)	0.0227 (2)
O4	1.23447 (12)	−0.12322 (10)	0.38559 (10)	0.01808 (19)
O5	0.84001 (12)	0.41637 (10)	0.63798 (10)	0.01381 (18)
H51	0.824 (2)	0.328 (2)	0.6383 (18)	0.026 (5)*
H52	0.880 (3)	0.466 (2)	0.710 (2)	0.033 (5)*
O6	1.09929 (14)	0.36688 (11)	−0.10135 (11)	0.0217 (2)
H61	1.060 (2)	0.3618 (18)	−0.0275 (19)	0.020*
H62	1.093 (2)	0.444 (2)	−0.1194 (17)	0.020*
N1	1.15013 (13)	0.35208 (11)	0.50331 (10)	0.0123 (2)
N2	1.00731 (15)	−0.08680 (12)	0.27740 (11)	0.0164 (2)
H21	0.955 (2)	−0.027 (2)	0.2615 (17)	0.021 (4)*
H22	0.976 (2)	−0.178 (2)	0.2312 (19)	0.028 (5)*
C1	0.86838 (16)	0.29893 (13)	0.22424 (12)	0.0132 (2)
C2	0.77440 (16)	0.14302 (13)	0.16204 (12)	0.0136 (2)
C3	0.65161 (17)	0.06356 (14)	0.23287 (13)	0.0166 (3)
H3	0.6270	0.1096	0.3197	0.020*
C4	0.56565 (17)	−0.08093 (14)	0.17828 (14)	0.0186 (3)
H4	0.4811	−0.1330	0.2268	0.022*

C5	0.60317 (17)	−0.15037 (14)	0.05176 (13)	0.0166 (3)
C6	0.72616 (18)	−0.07365 (14)	−0.01936 (13)	0.0193 (3)
H6	0.7531	−0.1207	−0.1049	0.023*
C7	0.80961 (18)	0.07279 (14)	0.03580 (13)	0.0178 (3)
H7	0.8920	0.1256	−0.0138	0.021*
C8	0.5467 (2)	−0.37024 (15)	−0.11975 (15)	0.0267 (3)
H8A	0.4740	−0.4712	−0.1386	0.040*
H8B	0.6672	−0.3705	−0.1161	0.040*
H8C	0.5229	−0.3223	−0.1922	0.040*
C9	1.30962 (17)	0.40473 (14)	0.56440 (13)	0.0165 (3)
H9	1.3474	0.5053	0.6080	0.020*
C10	1.42177 (17)	0.31926 (14)	0.56686 (14)	0.0191 (3)
H10	1.5328	0.3600	0.6130	0.023*
C11	1.36869 (17)	0.17315 (14)	0.50057 (13)	0.0156 (2)
H11	1.4428	0.1119	0.5007	0.019*
C12	1.20523 (16)	0.11758 (13)	0.43385 (12)	0.0124 (2)
C13	1.09960 (16)	0.21032 (13)	0.43965 (12)	0.0124 (2)
H13	0.9867	0.1717	0.3967	0.015*
C14	1.14890 (16)	−0.04076 (13)	0.36228 (12)	0.0132 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01171 (11)	0.00792 (11)	0.01082 (11)	0.00341 (8)	−0.00027 (8)	0.00012 (8)
O1	0.0145 (4)	0.0117 (4)	0.0131 (4)	0.0045 (3)	−0.0005 (3)	−0.0006 (3)
O2	0.0262 (5)	0.0119 (4)	0.0144 (4)	0.0005 (4)	0.0021 (4)	0.0015 (3)
O3	0.0265 (5)	0.0112 (4)	0.0244 (5)	−0.0007 (4)	−0.0025 (4)	−0.0016 (4)
O4	0.0195 (5)	0.0117 (4)	0.0246 (5)	0.0068 (4)	0.0026 (4)	0.0039 (4)
O5	0.0164 (4)	0.0100 (4)	0.0140 (4)	0.0034 (3)	−0.0002 (3)	0.0007 (3)
O6	0.0344 (6)	0.0147 (5)	0.0164 (5)	0.0076 (4)	0.0037 (4)	0.0025 (4)
N1	0.0140 (5)	0.0108 (5)	0.0123 (5)	0.0044 (4)	0.0013 (4)	0.0018 (4)
N2	0.0217 (6)	0.0112 (5)	0.0167 (5)	0.0071 (4)	−0.0002 (4)	0.0010 (4)
C1	0.0146 (6)	0.0117 (5)	0.0137 (6)	0.0052 (4)	−0.0024 (4)	0.0017 (4)
C2	0.0151 (6)	0.0112 (5)	0.0135 (6)	0.0039 (4)	−0.0024 (5)	0.0007 (4)
C3	0.0175 (6)	0.0152 (6)	0.0157 (6)	0.0043 (5)	0.0021 (5)	0.0006 (5)
C4	0.0174 (6)	0.0152 (6)	0.0211 (6)	0.0011 (5)	0.0022 (5)	0.0033 (5)
C5	0.0173 (6)	0.0111 (6)	0.0190 (6)	0.0025 (5)	−0.0049 (5)	0.0006 (5)
C6	0.0261 (7)	0.0152 (6)	0.0136 (6)	0.0041 (5)	0.0007 (5)	−0.0018 (5)
C7	0.0223 (6)	0.0139 (6)	0.0144 (6)	0.0016 (5)	0.0019 (5)	0.0014 (5)
C8	0.0364 (8)	0.0146 (6)	0.0236 (7)	0.0044 (6)	−0.0065 (6)	−0.0038 (5)
C9	0.0165 (6)	0.0115 (6)	0.0195 (6)	0.0036 (5)	−0.0013 (5)	−0.0002 (5)
C10	0.0140 (6)	0.0169 (6)	0.0250 (7)	0.0046 (5)	−0.0031 (5)	0.0013 (5)
C11	0.0161 (6)	0.0150 (6)	0.0185 (6)	0.0085 (5)	0.0029 (5)	0.0043 (5)
C12	0.0158 (6)	0.0104 (5)	0.0120 (5)	0.0044 (4)	0.0041 (4)	0.0034 (4)
C13	0.0140 (6)	0.0116 (5)	0.0117 (5)	0.0036 (4)	0.0014 (4)	0.0028 (4)
C14	0.0169 (6)	0.0110 (5)	0.0129 (5)	0.0047 (4)	0.0061 (5)	0.0037 (4)

Geometric parameters (Å, º)

Ni1—O1	2.0569 (9)	C2—C7	1.3904 (18)
Ni1—O1^{i}	2.0569 (9)	C3—C4	1.3822 (18)
Ni1—O5	2.0697 (9)	C3—H3	0.95
Ni1—O5^{i}	2.0697 (9)	C4—C5	1.3970 (19)
Ni1—N1	2.1167 (10)	C4—H4	0.95
Ni1—N1^{i}	2.1167 (10)	C5—C6	1.3902 (19)
O1—C1	1.2681 (15)	C6—C7	1.3941 (18)
O2—C1	1.2644 (16)	C6—H6	0.95
O3—C5	1.3607 (15)	C7—H7	0.95
O3—C8	1.4274 (18)	C8—H8A	0.98
O4—C14	1.2392 (15)	C8—H8B	0.98
O5—H51	0.83 (2)	C8—H8C	0.98
O5—H52	0.79 (2)	C9—C10	1.3858 (18)
O6—H61	0.823 (18)	C9—H9	0.95
O6—H62	0.818 (18)	C10—C11	1.3867 (18)
N1—C9	1.3421 (16)	C10—H10	0.95
N1—C13	1.3434 (15)	C11—C12	1.3913 (18)
N2—C14	1.3324 (17)	C11—H11	0.95
N2—H21	0.839 (18)	C12—C13	1.3910 (17)
N2—H22	0.877 (19)	C12—C14	1.5017 (16)
C1—C2	1.5001 (17)	C13—H13	0.95
C2—C3	1.3995 (18)		

O1^{i}—Ni1—O1	180.0	C3—C4—C5	119.95 (12)
O1—Ni1—O5	88.52 (4)	C3—C4—H4	120.0
O1^{i}—Ni1—O5	91.48 (4)	C5—C4—H4	120.0
O1—Ni1—O5^{i}	91.48 (4)	O3—C5—C4	115.16 (12)
O1^{i}—Ni1—O5^{i}	88.52 (4)	O3—C5—C6	124.95 (12)
O1—Ni1—N1	88.64 (4)	C6—C5—C4	119.89 (12)
O1^{i}—Ni1—N1	91.36 (4)	C5—C6—C7	119.52 (12)
O1—Ni1—N1^{i}	91.36 (4)	C5—C6—H6	120.2
O1^{i}—Ni1—N1^{i}	88.64 (4)	C7—C6—H6	120.2
O5—Ni1—O5^{i}	180.000 (1)	C2—C7—C6	121.20 (12)
O5—Ni1—N1	93.21 (4)	C2—C7—H7	119.4
O5^{i}—Ni1—N1	86.79 (4)	C6—C7—H7	119.4
O5—Ni1—N1^{i}	86.79 (4)	O3—C8—H8A	109.5
O5^{i}—Ni1—N1^{i}	93.21 (4)	O3—C8—H8B	109.5
N1—Ni1—N1^{i}	180.0	O3—C8—H8C	109.5
C1—O1—Ni1	130.22 (8)	H8A—C8—H8B	109.5
C5—O3—C8	117.74 (11)	H8A—C8—H8C	109.5
Ni1—O5—H51	117.6 (12)	H8B—C8—H8C	109.5
Ni1—O5—H52	104.9 (14)	N1—C9—C10	123.11 (12)
H51—O5—H52	111.1 (19)	N1—C9—H9	118.4
H62—O6—H61	108.0 (17)	C10—C9—H9	118.4
C9—N1—Ni1	118.24 (8)	C9—C10—C11	118.69 (12)
C9—N1—C13	117.80 (11)	C9—C10—H10	120.7

C13—N1—Ni1	123.79 (8)	C11—C10—H10	120.7
C14—N2—H21	120.0 (12)	C10—C11—C12	118.98 (11)
C14—N2—H22	119.6 (12)	C10—C11—H11	120.5
H21—N2—H22	120.1 (17)	C12—C11—H11	120.5
O1—C1—C2	116.29 (11)	C11—C12—C14	118.60 (11)
O2—C1—O1	124.22 (11)	C13—C12—C11	118.44 (11)
O2—C1—C2	119.46 (11)	C13—C12—C14	122.93 (11)
C3—C2—C1	120.07 (11)	N1—C13—C12	122.95 (11)
C7—C2—C1	121.44 (12)	N1—C13—H13	118.5
C7—C2—C3	118.47 (11)	C12—C13—H13	118.5
C2—C3—H3	119.5	O4—C14—N2	122.82 (12)
C4—C3—C2	120.95 (12)	O4—C14—C12	118.87 (11)
C4—C3—H3	119.5	N2—C14—C12	118.31 (11)
O5—Ni1—O1—C1	−160.75 (10)	C1—C2—C3—C4	−178.93 (12)
O5^{i}—Ni1—O1—C1	19.25 (10)	C7—C2—C3—C4	−0.71 (19)
N1—Ni1—O1—C1	−67.50 (10)	C1—C2—C7—C6	177.72 (12)
N1^{i}—Ni1—O1—C1	112.50 (10)	C3—C2—C7—C6	−0.5 (2)
O1—Ni1—N1—C9	162.56 (10)	C2—C3—C4—C5	1.2 (2)
O1^{i}—Ni1—N1—C9	−17.44 (10)	C8—O3—C5—C4	−178.85 (12)
O1—Ni1—N1—C13	−12.62 (10)	C8—O3—C5—C6	1.3 (2)
O1^{i}—Ni1—N1—C13	167.38 (10)	C3—C4—C5—O3	179.75 (12)
O5—Ni1—N1—C9	−109.01 (10)	C3—C4—C5—C6	−0.4 (2)
O5^{i}—Ni1—N1—C9	70.99 (10)	O3—C5—C6—C7	179.07 (13)
O5—Ni1—N1—C13	75.81 (10)	C4—C5—C6—C7	−0.7 (2)
O5^{i}—Ni1—N1—C13	−104.19 (10)	C5—C6—C7—C2	1.2 (2)
Ni1—O1—C1—O2	−29.75 (18)	N1—C9—C10—C11	1.5 (2)
Ni1—O1—C1—C2	148.20 (9)	C9—C10—C11—C12	0.1 (2)
Ni1—N1—C9—C10	−176.80 (10)	C10—C11—C12—C13	−1.78 (19)
C13—N1—C9—C10	−1.33 (19)	C10—C11—C12—C14	179.97 (11)
Ni1—N1—C13—C12	174.71 (9)	C11—C12—C13—N1	2.04 (18)
C9—N1—C13—C12	−0.49 (18)	C14—C12—C13—N1	−179.79 (11)
O1—C1—C2—C3	6.12 (17)	C11—C12—C14—O4	13.48 (17)
O1—C1—C2—C7	−172.05 (12)	C11—C12—C14—N2	−167.30 (12)
O2—C1—C2—C3	−175.83 (11)	C13—C12—C14—O4	−164.68 (12)
O2—C1—C2—C7	6.00 (18)	C13—C12—C14—N2	14.53 (18)

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H22···O6^{ii}	0.88 (2)	1.96 (2)	2.8306 (16)	170 (2)
O5—H51···O4^{iii}	0.83 (2)	1.88 (2)	2.7074 (14)	171 (2)
O5—H52···O2^{i}	0.79 (2)	1.95 (2)	2.7040 (14)	159 (2)
O6—H61···O2	0.82 (2)	1.99 (2)	2.8136 (14)	174 (2)
O6—H62···O2^{iv}	0.82 (2)	2.08 (2)	2.8887 (15)	169 (2)

C9—H9···O1^{i}	0.95	2.35	2.9719 (16)	123
C10—H10···O5^{v}	0.95	2.41	3.2973 (17)	156

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