

Poly[aqua[μ_2 -1,1'-(butane-1,4-diyl)-diimidazole](μ_2 -naphthalene-1,4-dicarboxylato)nickel(II)]

Xian-Zhi Zou

Department of Chemistry, College of Chemistry and Biology, Beihua University, Jilin City 132013, People's Republic of China

Correspondence e-mail: jlsxzz@126.com

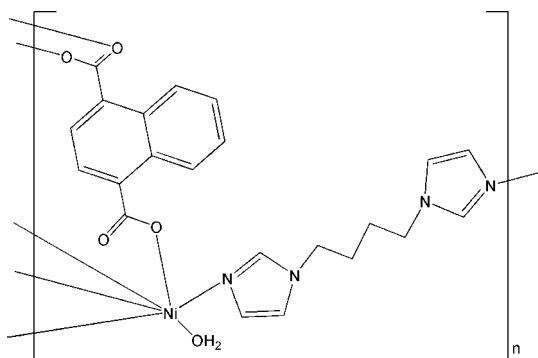
Received 24 July 2008; accepted 29 July 2008

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.050; wR factor = 0.097; data-to-parameter ratio = 14.0.

In the title compound, $[\text{Ni}(\text{C}_{12}\text{H}_6\text{O}_4)(\text{C}_{10}\text{H}_{14}\text{N}_4)(\text{H}_2\text{O})]_n$, the coordination polyhedron around each Ni^{II} atom is a distorted *cis*- NiN_2O_4 octahedron. The naphthalene-1,4-dicarboxylate and 1,1'-(butane-1,4-diyl)diimidazole ligands bridge the Ni centres to form a two-dimensional (4,4)-network, and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds complete the structure.

Related literature

For general background, see: Batten & Robson (1998). For a related structure, see: Ma *et al.*, (2003).



Experimental

Crystal data

$[\text{Ni}(\text{C}_{12}\text{H}_6\text{O}_4)(\text{C}_{10}\text{H}_{14}\text{N}_4)(\text{H}_2\text{O})]$

$M_r = 481.15$

Monoclinic, $P2_1/n$

$a = 12.4213$ (12) Å

$b = 13.2543$ (13) Å

$c = 13.4328$ (13) Å

$\beta = 107.361$ (2)°

$V = 2110.8$ (4) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 0.96$ mm⁻¹

$T = 293$ (2) K

$0.19 \times 0.17 \times 0.15$ mm

Data collection

Bruker APEX CCD diffractometer

Absorption correction: multi-scan

(*SADABS*; Bruker, 1998)

$T_{\text{min}} = 0.827$, $T_{\text{max}} = 0.866$

11720 measured reflections

4157 independent reflections

2982 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.063$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.097$

$S = 1.05$

4157 reflections

297 parameters

3 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 0.54$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.40$ e Å⁻³

Table 1

Selected bond lengths (Å).

Ni1—O1W	2.125 (2)	Ni1—O3 ⁱ	2.347 (2)
Ni1—O2	2.040 (2)	Ni1—N1	2.060 (3)
Ni1—O1 ⁱ	2.116 (2)	Ni1—N4 ⁱⁱ	2.099 (3)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O1W—HW12 \cdots O1 ⁱⁱⁱ	0.819 (16)	1.847 (18)	2.661 (3)	172 (3)
O1W—HW11 \cdots O4	0.83 (4)	1.83 (4)	2.651 (3)	169 (3)

Symmetry code: (iii) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The author thanks Beihua University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2770).

References

- Batten, S. R. & Robson, R. (1998). *Angew. Chem. Int. Ed.* **37**, 1460–1494.
- Bruker (1998). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Ma, J.-F., Yang, J., Zheng, G.-L., Li, L. & Liu, J.-F. (2003). *Inorg. Chem.* **42**, 7531–7534.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2008). E64, m1105 [doi:10.1107/S1600536808024008]

Poly[aqua[μ_2 -1,1'-(butane-1,4-diyl)diimidazole](μ_2 -naphthalene-1,4-dicarboxylato)nickel(II)]

X.-Z. Zou

Comment

Metal-organic frameworks are currently of great interest because of their interesting structures and potential applications. So far, some interesting interpenetrated or entangled metal-organic networks with bis(imidazole)-containing ligands have been documented (Batten & Robson, 1998). Flexible ligands such as 1,1'-(1,4-butanediyl)bis(imidazole) (*L*) have been less explored to date (Ma *et al.*, 2003). In this work, we selected 1,4-naphthalenedicarboxylic acid (H_2ndc) and *L* as linkers, generating a new coordination polymer, $[Ni(ndc)(L)(H_2O)]$, (I), which is reported here.

In compound (I) each Ni^{II} atom is six-coordinated by two N atoms from two different *L* ligands, and four O atoms from three carboxylate oxygen atoms (one bidentate, one monodentate) and one water molecule in a distorted cis- NiN_2O_4 octohedral coordination sphere (Fig. 1). The two neighbouring Ni^{II} atoms are bridged by the *ndc* and *L* ligands to form a two-dimensional (4,4) network (Fig. 2) and O—H \cdots O hydrogen bonds arising from the water molecule (Table 2) complete the structure.

Experimental

A mixture of H_2ndc (0.5 mmol), *L* (0.5 mmol), NaOH (1 mmol) and $NiCl_2 \cdot 6H_2O$ (0.5 mmol) was suspended in 12 ml of deionized water and sealed in a 20-ml Teflon-lined autoclave. Upon heating at 433 K for one week, the autoclave was slowly cooled to room temperature. Green blocks of (I) were collected, washed with deionized water and dried.

Refinement

The H atoms on C atoms were generated geometrically and refined as riding with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The water H atoms were located in a difference Fourier map and refined with the O—H distance restrained to 0.85 ± 0.01 Å.

Figures

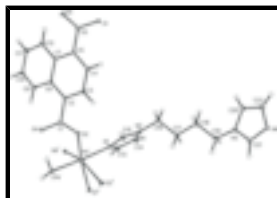


Fig. 1. The structure of (I), with displacement ellipsoids for the non-hydrogen atoms drawn at the 30% probability level. Symmetry codes: (i) $x, y - 1, z$; (ii) $1/2 + x, 0.5 - y, z - 1/2$.



Fig. 2. View of part of the polymeric layer structure of (I).

Poly[aqua[μ_2 -1,1'-(butane-1,4-diyl)diimidazole](μ_2 -naphthalene-1,4-dicarboxylato)nickel(II)]

Crystal data

[Ni(C₁₂H₆O₄)(C₁₀H₁₄N₄)(H₂O)]

$M_r = 481.15$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 12.4213$ (12) Å

$b = 13.2543$ (13) Å

$c = 13.4328$ (13) Å

$\beta = 107.361$ (2)°

$V = 2110.8$ (4) Å³

$Z = 4$

$F_{000} = 1000$

$D_x = 1.514$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 4157 reflections

$\theta = 1.9$ – 26.1 °

$\mu = 0.96$ mm⁻¹

$T = 293$ (2) K

Block, green

$0.19 \times 0.17 \times 0.15$ mm

Data collection

Bruker APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 1998)

$T_{\min} = 0.827$, $T_{\max} = 0.866$

11720 measured reflections

4157 independent reflections

2982 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.063$

$\theta_{\max} = 26.1$ °

$\theta_{\min} = 2.0$ °

$h = -9 \rightarrow 15$

$k = -16 \rightarrow 14$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.097$

$S = 1.05$

4157 reflections

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

$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.54$ e Å⁻³

297 parameters

$$\Delta\rho_{\min} = -0.40 \text{ e } \text{\AA}^{-3}$$

3 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2969 (3)	0.1196 (2)	0.2222 (3)	0.0208 (8)
C2	0.2145 (3)	0.1584 (2)	0.2758 (2)	0.0190 (8)
C3	0.2114 (3)	0.2586 (2)	0.2946 (3)	0.0264 (9)
H3	0.2583	0.3019	0.2721	0.032*
C4	0.1392 (3)	0.2986 (2)	0.3472 (3)	0.0238 (8)
H4	0.1399	0.3677	0.3597	0.029*
C5	0.0674 (3)	0.2376 (2)	0.3805 (2)	0.0203 (8)
C6	-0.0034 (3)	0.2829 (2)	0.4420 (3)	0.0218 (8)
C7	0.0636 (3)	0.1328 (2)	0.3576 (2)	0.0180 (7)
C8	0.1382 (3)	0.0919 (2)	0.3055 (2)	0.0172 (7)
C9	0.1306 (3)	-0.0118 (2)	0.2806 (3)	0.0256 (8)
H9	0.1795	-0.0393	0.2473	0.031*
C10	0.0536 (3)	-0.0723 (3)	0.3042 (3)	0.0281 (9)
H10	0.0497	-0.1404	0.2868	0.034*
C11	-0.0196 (3)	-0.0320 (3)	0.3546 (3)	0.0312 (9)
H11	-0.0722	-0.0738	0.3706	0.037*
C12	-0.0157 (3)	0.0664 (2)	0.3806 (3)	0.0257 (8)
H12	-0.0657	0.0914	0.4141	0.031*
C13	0.1710 (3)	0.2460 (3)	-0.1581 (3)	0.0335 (10)
H13	0.1644	0.1937	-0.2056	0.040*
C14	0.1151 (4)	0.3340 (3)	-0.1787 (3)	0.0430 (11)
H14	0.0644	0.3537	-0.2418	0.052*
C15	0.2219 (3)	0.3312 (3)	-0.0198 (3)	0.0310 (9)
H15	0.2581	0.3510	0.0484	0.037*
C16	0.1118 (3)	0.4914 (2)	-0.0714 (3)	0.0274 (9)
H16A	0.1268	0.5024	0.0029	0.033*
H16B	0.0311	0.4976	-0.1039	0.033*
C17	0.1715 (3)	0.5711 (2)	-0.1149 (3)	0.0296 (9)
H17A	0.1498	0.5648	-0.1903	0.036*

supplementary materials

H17B	0.2523	0.5605	-0.0882	0.036*
C18	0.1434 (3)	0.6771 (2)	-0.0863 (3)	0.0293 (9)
H18A	0.0622	0.6862	-0.1083	0.035*
H18B	0.1705	0.6855	-0.0112	0.035*
C19	0.1971 (3)	0.7560 (2)	-0.1379 (3)	0.0293 (9)
H19A	0.2754	0.7381	-0.1277	0.035*
H19B	0.1590	0.7559	-0.2123	0.035*
C20	0.1050 (3)	0.9021 (3)	-0.0704 (3)	0.0395 (11)
H20	0.0353	0.8734	-0.0749	0.047*
C21	0.2746 (3)	0.9270 (2)	-0.0777 (3)	0.0238 (8)
H21	0.3436	0.9163	-0.0898	0.029*
N4	0.2477 (2)	1.01080 (19)	-0.0399 (2)	0.0212 (7)
C23	0.1402 (3)	0.9948 (3)	-0.0365 (3)	0.0378 (10)
H23	0.0973	1.0419	-0.0137	0.045*
N1	0.2384 (2)	0.2446 (2)	-0.0581 (2)	0.0224 (7)
N2	0.1476 (2)	0.38862 (19)	-0.0887 (2)	0.0232 (7)
N3	0.1920 (2)	0.8579 (2)	-0.0970 (2)	0.0240 (7)
O1	-0.05860 (18)	0.36339 (16)	0.40707 (17)	0.0227 (5)
O2	0.3062 (2)	0.17401 (16)	0.14730 (18)	0.0266 (6)
O1W	0.4733 (2)	0.04150 (17)	0.12115 (19)	0.0208 (6)
O3	-0.00731 (19)	0.24467 (16)	0.52507 (17)	0.0265 (6)
O4	0.35191 (19)	0.04171 (16)	0.25344 (18)	0.0257 (6)
Ni1	0.35134 (4)	0.13565 (3)	0.01819 (3)	0.02231 (14)
HW12	0.495 (2)	-0.0135 (16)	0.107 (2)	0.020 (10)*
HW11	0.440 (3)	0.034 (2)	0.166 (2)	0.053 (15)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.023 (2)	0.0180 (19)	0.0236 (19)	-0.0040 (15)	0.0094 (15)	-0.0067 (15)
C2	0.025 (2)	0.0174 (19)	0.0172 (18)	0.0032 (14)	0.0099 (15)	0.0011 (14)
C3	0.034 (2)	0.0166 (19)	0.037 (2)	-0.0033 (16)	0.0226 (18)	0.0027 (16)
C4	0.033 (2)	0.0108 (18)	0.033 (2)	0.0005 (15)	0.0184 (18)	-0.0043 (15)
C5	0.024 (2)	0.0201 (19)	0.0198 (19)	0.0018 (15)	0.0110 (15)	0.0017 (15)
C6	0.023 (2)	0.0178 (19)	0.028 (2)	-0.0063 (15)	0.0133 (17)	-0.0083 (16)
C7	0.0207 (18)	0.0162 (18)	0.0187 (17)	0.0009 (14)	0.0085 (14)	0.0007 (14)
C8	0.0238 (19)	0.0136 (17)	0.0162 (17)	0.0012 (14)	0.0088 (15)	0.0009 (13)
C9	0.030 (2)	0.021 (2)	0.030 (2)	0.0018 (16)	0.0157 (17)	-0.0013 (16)
C10	0.034 (2)	0.0147 (19)	0.039 (2)	-0.0018 (16)	0.0167 (19)	-0.0041 (16)
C11	0.037 (2)	0.022 (2)	0.041 (2)	-0.0094 (17)	0.021 (2)	-0.0018 (17)
C12	0.030 (2)	0.025 (2)	0.028 (2)	-0.0024 (16)	0.0182 (17)	-0.0027 (16)
C13	0.047 (3)	0.023 (2)	0.029 (2)	0.0090 (18)	0.0076 (19)	-0.0050 (17)
C14	0.057 (3)	0.035 (2)	0.026 (2)	0.019 (2)	-0.004 (2)	0.0003 (18)
C15	0.035 (2)	0.024 (2)	0.027 (2)	0.0056 (17)	-0.0011 (18)	-0.0046 (16)
C16	0.027 (2)	0.019 (2)	0.037 (2)	0.0056 (15)	0.0124 (18)	-0.0005 (16)
C17	0.030 (2)	0.020 (2)	0.039 (2)	0.0018 (16)	0.0105 (18)	-0.0001 (17)
C18	0.029 (2)	0.020 (2)	0.039 (2)	0.0005 (16)	0.0105 (18)	0.0004 (17)
C19	0.033 (2)	0.020 (2)	0.036 (2)	-0.0053 (16)	0.0123 (18)	-0.0043 (17)

C20	0.025 (2)	0.025 (2)	0.074 (3)	-0.0038 (17)	0.023 (2)	-0.005 (2)
C21	0.019 (2)	0.024 (2)	0.031 (2)	-0.0005 (15)	0.0100 (16)	0.0025 (16)
N4	0.0213 (17)	0.0140 (15)	0.0293 (17)	-0.0003 (12)	0.0092 (13)	-0.0001 (13)
C23	0.025 (2)	0.023 (2)	0.071 (3)	-0.0001 (17)	0.023 (2)	-0.011 (2)
N1	0.0244 (17)	0.0182 (16)	0.0264 (17)	0.0042 (12)	0.0104 (14)	0.0006 (13)
N2	0.0265 (17)	0.0127 (16)	0.0304 (17)	0.0036 (12)	0.0086 (14)	0.0024 (12)
N3	0.0238 (17)	0.0149 (16)	0.0341 (17)	-0.0021 (13)	0.0099 (14)	-0.0015 (13)
O1	0.0282 (14)	0.0136 (12)	0.0333 (14)	0.0018 (10)	0.0196 (11)	0.0008 (11)
O2	0.0385 (16)	0.0226 (14)	0.0284 (14)	0.0093 (11)	0.0246 (12)	0.0068 (11)
O1W	0.0230 (15)	0.0157 (14)	0.0277 (15)	0.0028 (11)	0.0138 (12)	-0.0024 (11)
O3	0.0388 (16)	0.0215 (13)	0.0276 (14)	0.0028 (11)	0.0226 (12)	0.0014 (11)
O4	0.0309 (15)	0.0202 (14)	0.0316 (14)	0.0091 (11)	0.0178 (12)	0.0062 (11)
Ni1	0.0259 (3)	0.0180 (2)	0.0269 (3)	0.0016 (2)	0.0137 (2)	0.0008 (2)

Geometric parameters (Å, °)

C1—O4	1.240 (4)	C16—C17	1.505 (5)
C1—O2	1.270 (4)	C16—H16A	0.9700
C1—C2	1.508 (4)	C16—H16B	0.9700
C2—C3	1.356 (4)	C17—C18	1.525 (4)
C2—C8	1.434 (4)	C17—H17A	0.9700
C3—C4	1.400 (4)	C17—H17B	0.9700
C3—H3	0.9300	C18—C19	1.515 (4)
C4—C5	1.375 (4)	C18—H18A	0.9700
C4—H4	0.9300	C18—H18B	0.9700
C5—C7	1.420 (4)	C19—N3	1.466 (4)
C5—C6	1.500 (4)	C19—H19A	0.9700
C6—O3	1.240 (4)	C19—H19B	0.9700
C6—O1	1.279 (4)	C20—C23	1.338 (5)
C7—C12	1.421 (4)	C20—N3	1.368 (4)
C7—C8	1.424 (4)	C20—H20	0.9300
C8—C9	1.412 (4)	C21—N4	1.306 (4)
C9—C10	1.356 (4)	C21—N3	1.341 (4)
C9—H9	0.9300	C21—H21	0.9300
C10—C11	1.392 (5)	N4—C23	1.367 (4)
C10—H10	0.9300	N4—Ni1 ⁱ	2.099 (3)
C11—C12	1.347 (4)	C23—H23	0.9300
C11—H11	0.9300	O1—Ni1 ⁱⁱ	2.116 (2)
C12—H12	0.9300	O1W—HW12	0.819 (16)
C13—C14	1.343 (5)	O1W—HW11	0.83 (4)
C13—N1	1.355 (4)	O3—Ni1 ⁱⁱ	2.347 (2)
C13—H13	0.9300	Ni1—O1W	2.125 (2)
C14—N2	1.363 (4)	Ni1—O2	2.040 (2)
C14—H14	0.9300	Ni1—O1 ⁱⁱⁱ	2.116 (2)
C15—N1	1.299 (4)	Ni1—O3 ⁱⁱⁱ	2.347 (2)
C15—N2	1.334 (4)	Ni1—N1	2.060 (3)
C15—H15	0.9300	Ni1—N4 ^{iv}	2.099 (3)
C16—N2	1.472 (4)		

supplementary materials

O4—C1—O2	124.8 (3)	H17A—C17—H17B	107.9
O4—C1—C2	120.4 (3)	C19—C18—C17	110.8 (3)
O2—C1—C2	114.8 (3)	C19—C18—H18A	109.5
C3—C2—C8	119.5 (3)	C17—C18—H18A	109.5
C3—C2—C1	118.9 (3)	C19—C18—H18B	109.5
C8—C2—C1	121.5 (3)	C17—C18—H18B	109.5
C2—C3—C4	121.6 (3)	H18A—C18—H18B	108.1
C2—C3—H3	119.2	N3—C19—C18	113.0 (3)
C4—C3—H3	119.2	N3—C19—H19A	109.0
C5—C4—C3	121.1 (3)	C18—C19—H19A	109.0
C5—C4—H4	119.5	N3—C19—H19B	109.0
C3—C4—H4	119.5	C18—C19—H19B	109.0
C4—C5—C7	119.2 (3)	H19A—C19—H19B	107.8
C4—C5—C6	119.1 (3)	C23—C20—N3	106.2 (3)
C7—C5—C6	121.7 (3)	C23—C20—H20	126.9
O3—C6—O1	120.7 (3)	N3—C20—H20	126.9
O3—C6—C5	121.2 (3)	N4—C21—N3	112.7 (3)
O1—C6—C5	118.1 (3)	N4—C21—H21	123.6
C5—C7—C12	122.5 (3)	N3—C21—H21	123.6
C5—C7—C8	119.6 (3)	C21—N4—C23	104.3 (3)
C12—C7—C8	117.8 (3)	C21—N4—Ni ⁱ	128.0 (2)
C9—C8—C7	118.6 (3)	C23—N4—Ni ⁱ	127.4 (2)
C9—C8—C2	122.4 (3)	C20—C23—N4	110.8 (3)
C7—C8—C2	118.9 (3)	C20—C23—H23	124.6
C10—C9—C8	121.5 (3)	N4—C23—H23	124.6
C10—C9—H9	119.2	C15—N1—C13	104.8 (3)
C8—C9—H9	119.2	C15—N1—Ni ⁱ	126.0 (2)
C9—C10—C11	119.7 (3)	C13—N1—Ni ⁱ	129.1 (2)
C9—C10—H10	120.2	C15—N2—C14	105.8 (3)
C11—C10—H10	120.2	C15—N2—C16	126.7 (3)
C12—C11—C10	121.3 (3)	C14—N2—C16	127.5 (3)
C12—C11—H11	119.4	C21—N3—C20	106.0 (3)
C10—C11—H11	119.4	C21—N3—C19	125.8 (3)
C11—C12—C7	121.1 (3)	C20—N3—C19	128.1 (3)
C11—C12—H12	119.5	C6—O1—Ni ⁱⁱ	94.87 (19)
C7—C12—H12	119.5	C1—O2—Ni ⁱ	130.1 (2)
C14—C13—N1	110.2 (3)	Ni ⁱ —O1W—HW12	126 (2)
C14—C13—H13	124.9	Ni ⁱ —O1W—HW11	97 (3)
N1—C13—H13	124.9	HW12—O1W—HW11	110 (2)
C13—C14—N2	106.3 (3)	C6—O3—Ni ⁱⁱ	85.3 (2)
C13—C14—H14	126.9	O2—Ni ⁱ —N1	85.93 (10)
N2—C14—H14	126.9	O2—Ni ⁱ —N4 ^{iv}	102.65 (10)
N1—C15—N2	112.9 (3)	N1—Ni ⁱ —N4 ^{iv}	96.70 (11)
N1—C15—H15	123.6	O2—Ni ⁱ —O1 ⁱⁱⁱ	159.34 (9)
N2—C15—H15	123.6	N1—Ni ⁱ —O1 ⁱⁱⁱ	94.01 (10)
N2—C16—C17	112.4 (3)	N4 ^{iv} —Ni ⁱ —O1 ⁱⁱⁱ	97.87 (10)
N2—C16—H16A	109.1	O2—Ni ⁱ —O1W	85.20 (9)

C17—C16—H16A	109.1	N1—Ni1—O1W	169.33 (10)
N2—C16—H16B	109.1	N4 ^{iv} —Ni1—O1W	91.03 (10)
C17—C16—H16B	109.1	O1 ⁱⁱⁱ —Ni1—O1W	92.20 (9)
H16A—C16—H16B	107.9	O2—Ni1—O3 ⁱⁱⁱ	100.97 (9)
C16—C17—C18	111.9 (3)	N1—Ni1—O3 ⁱⁱⁱ	86.35 (10)
C16—C17—H17A	109.2	N4 ^{iv} —Ni1—O3 ⁱⁱⁱ	156.33 (9)
C18—C17—H17A	109.2	O1 ⁱⁱⁱ —Ni1—O3 ⁱⁱⁱ	58.47 (8)
C16—C17—H17B	109.2	O1W—Ni1—O3 ⁱⁱⁱ	89.53 (8)
C18—C17—H17B	109.2		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—HW12 \cdots O1 ^v	0.819 (16)	1.847 (18)	2.661 (3)	172 (3)
O1W—HW11 \cdots O4	0.83 (4)	1.83 (4)	2.651 (3)	169 (3)

Symmetry codes: (v) $-x+1/2, y-1/2, -z+1/2$.

Fig. 1

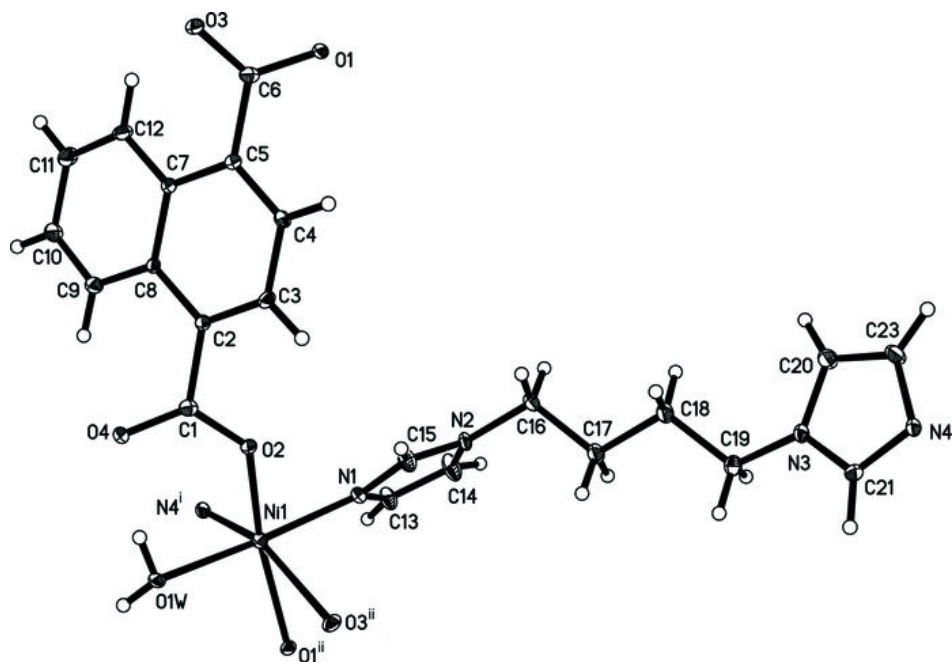


Fig. 2

