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# Poly[aqua[$\mu_3$-4-carboxy-2-(pyridin-4-yl)-1*H*-imidazole-5-carboxylato-$\kappa^5N^1,O^5:N^3,O^4:N^2$]nickel(II)]

**Xue-Min Jing,[a]* Shu-zhe Gong[b] and Li-Wei Xiao[a]**

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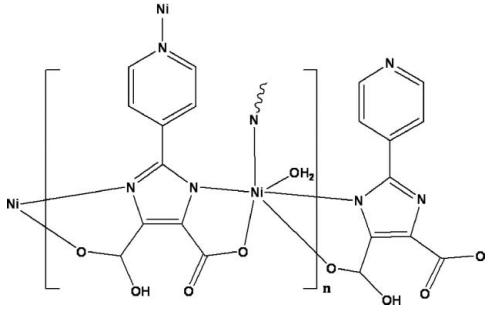
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.051; $wR$ factor = 0.118; data-to-parameter ratio = 11.9.

The water-coordinated $Ni^{2+}$ cation in the title compound, $[Ni(C_{10}H_5N_3O_4)(H_2O)]_n$, assumes an octahedral $NiN_3O_3$ coordination mode and is *N*,*O*-chelated by two deprotonated 2-(pyridin-4-yl)-1*H*-imidazole-4,5-dicarboxylic acid ($HPyImDC^{2-}$) ligands, forming a layer structure extending in the *bc* plane. The chains are arranged along the *b*-axis direction, forming a layer structure extending in the *bc* plane. O—H···O hydrogen bonding between the layers results in the formation of a three-dimensional supramolecular framework. The structure is isotypic with the Zn analogue [Li *et al.* (2009). *Cryst. Growth Des.* **6**, 3423–3431].

## Related literature

For the isotypic Zn compound, see: Li *et al.* (2009). The $HPyImDC^{2-}$ anion behaves as a T-shaped linker, see: Jing *et al.* (2010).




## Experimental

### Crystal data

$[Ni(C_{10}H_5N_3O_4)(H_2O)]$
$M_r$ = 307.88
Monoclinic, $P2_1/c$
$a$ = 7.5117 (15) Å
$b$ = 11.400 (2) Å
$c$ = 12.896 (4) Å
$\beta$ = 109.04 (3)°
$V$ = 1043.9 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.88 mm$^{-1}$
$T$ = 293 K
0.21 × 0.16 × 0.13 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.216, $T_{max}$ = 0.422
10075 measured reflections
2377 independent reflections
1951 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.067

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.118
$S$ = 1.04
2377 reflections
200 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.09 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O3 | 0.94 (7) | 1.57 (7) | 2.501 (4) | 171 (7) |
| O1$W$—H1$A$···O3$^{i}$ | 0.78 (9) | 1.95 (9) | 2.726 (5) | 174 (9) |
| O1$W$—H1$B$···O1$^{ii}$ | 0.73 (6) | 2.35 (6) | 3.007 (5) | 150 (5) |

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HP2024).

## References

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Jing, X., Meng, H., Li, G., Yu, Y., Huo, Q., Eddaoudi, M. & Liu, Y. (2010). *Cryst. Growth Des.* **10**, 3489–3495.
Li, X., Wu, B., Niu, C., Niu, Y. & Zhang, H. (2009). *Cryst. Growth Des.* **9**, 3423–3431.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2012). E**68**, m187 [doi:10.1107/S1600536812001900]

## Poly[aqua[$\mu_3$-4-carboxy-2-(pyridin-4-yl)-1*H*-imidazole-5-carboxylato-$\kappa^5N^1,O^5:N^3,O^4:N^2$]nickel(II)]

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### S1. Comment

Li *et al.* (2009) described the structure of [Zn($C_{10}H_5N_3O_4$)$H_2O$] as a stairway-like two-dimensional 3,3-connected layer held together *via* hydrogen-bonding interactions involving the carboxylic acid and water H atoms to be a three-dimensional network. The $HPyImDC^{2-}$ anion behaves as a T-shaped linker (Jing *et al.*, 2010) with one N atoms and bis-N,*O*-bridging modes chelating the Ni(II) atoms. The present centrosymmetric Ni analogue, (Fig. 1) is isomorphous, the two compounds having nearly identical unit-cell parameters.

As shown in Fig. 2a, the {$NiN_3O_3$} octahedra connect with the T-shaped $HPyImDC^{2-}$ anions to be a one-dimensional chain structure extending in the c direction. Then these one-dimensional chains arrange along the b direction to be a two-dimensional layer structure extending in the *bc* plane (Fig. 2 b), which are further connected through the hydrogen bonds occurred between O(1 W)—H(1 A)···O(3) (-*x* + 1,-*y*,-*z*) and O(1 W)—H(1B)···O(1)(*x*-1, *y*, *z*), respectively, to construct a three-dimensional supramolecular framework (Fig. 2c and Table 1).

### S2. Experimental

Preparation of the complex.

A solution of $NiCl_26H_2O$ (0.012 g, 0.5 mmol) and $H_3PyImDC$ (0.012 g, 0.05 mmol) in DMF (1 ml) and $H_2O$ (0.5 ml) was sealed into a 15 ml Teflon-lined stainless autoclave and heated at 433 K for 4 days and then cooled to room temperature gradually to afford well formed green block crystals in about 60% yield (based on Zn). Elemental analysis found (%): C, 39.06; H, 2.30; N, 13.72; Ni, 19.01. $H_7C_{10}N_3O_5Ni$ requires (%): C, 39.01; H, 2.29; N, 13.65; Ni, 19.06. IR (KBr, $cm^{-1}$): 3571 (*s*), 3083 (*m*), 2560 (w), 1675 (w), 1565 (*versus*), 1271 (*s*), 842 (*m*), 567 (w).

### S3. Refinement

The H atoms bonded to C were positioned geometrically with C—H distance 0.93–0.96 Å, and treated as riding atoms, with $U_{iso}$(H)=1.1Ueq(C). The H atoms bonded to O were located in a difference Fourier map and refined isotropically.

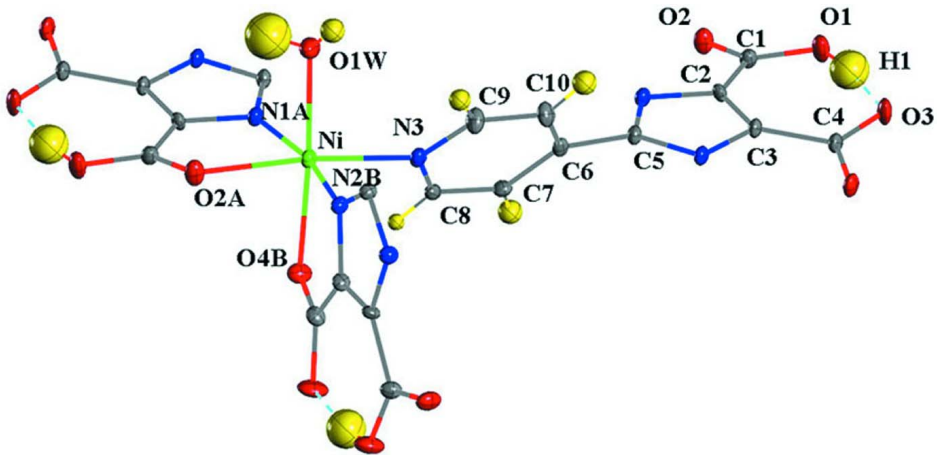


**Figure 1**

A view of the centrosymmetric molecule of (I), with displacement ellipsoids drawn at the 25% probability level [symmetry code: (i) -*x*, -*y* - 1, -*z*; (ii) *x*, -*y* - 1/2, *z* + 1/2; (iii) *x*, -*y* - 1/2, *z* - 1/2]

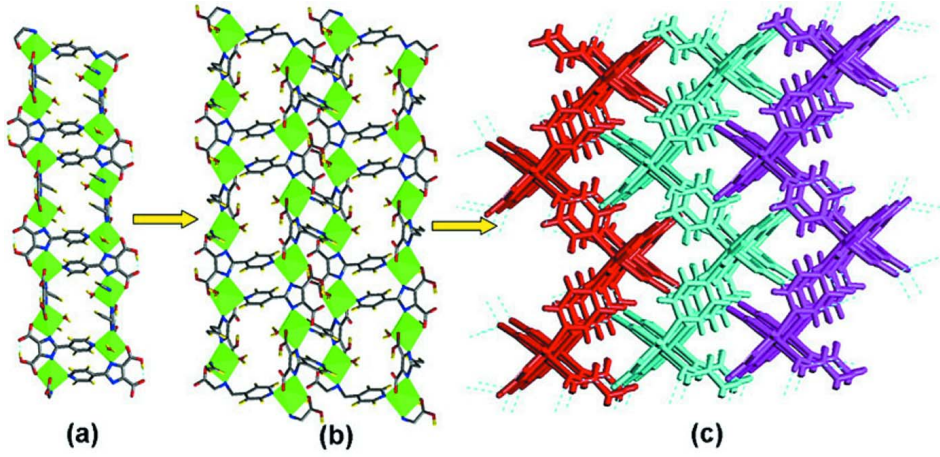


**Figure 2**

(*a*) A view showing the one-dimensional (one-dimensional) chain along the c direction; (*b*) one-dimensional chains arranged in the b direction to be a two-dimensional layer structure; (*c*) the two-dimensional layers packed in an AAA way *via* hydrogen-bonding interactions to be a three-dimensional network.

**Poly[aqua[$\mu_3$-4-carboxy-2-(pyridin-4-yl)-1*H*-imidazole-5-carboxylato-$\kappa^5N^1,O^5:N^3,O^4:N^2$]nickel(II)]**

*Crystal data*

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$c$ = 12.896 (4) Å
$\beta$ = 109.04 (3)°
$V$ = 1043.9 (4) Å$^3$
$Z$ = 4
$F(000)$ = 624
$D_x$ = 1.959 Mg m$^{-3}$
Melting point: not measured K
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2377 reflections
$\theta$ = 3.3–27.4°
$\mu$ = 1.88 mm$^{-1}$
$T$ = 293 K
Block, green
0.21 × 0.16 × 0.13 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9.00cm pixels $mm^{-1}$
phi and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.216, $T_{max}$ = 0.422
10075 measured reflections
2377 independent reflections
1951 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.067
$\theta_{max}$ = 27.4°, $\theta_{min}$ = 3.3°
$h$ = −9→9
$k$ = −14→14
$l$ = −16→16

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.118
$S$ = 1.04
2377 reflections
200 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
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 3.3079P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.55 e $Å^{-3}$
$\Delta\rho_{min}$ = −1.09 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 | 0.32031 (7) | −0.26730 (4) | 0.18242 (4) | 0.01465 (17) |
| O1 | 0.7267 (4) | −0.0698 (3) | 0.1164 (3) | 0.0285 (7) |
| H1 | 0.740 (10) | −0.063 (6) | 0.046 (6) | 0.08 (2)* |
| O2 | 0.5375 (4) | −0.1450 (3) | 0.1996 (2) | 0.0234 (7) |
| O3 | 0.7296 (4) | −0.0603 (3) | −0.0768 (2) | 0.0275 (7) |
| O4 | 0.5464 (4) | −0.1211 (2) | −0.2426 (2) | 0.0210 (6) |
| O1W | 0.1140 (5) | −0.1417 (3) | 0.1203 (3) | 0.0243 (7) |
| H1A | 0.163 (12) | −0.087 (8) | 0.106 (7) | 0.11 (3)* |
| H1B | 0.041 (8) | −0.120 (5) | 0.142 (4) | 0.030 (16)* |
| N1 | 0.3422 (5) | −0.2756 (3) | 0.0217 (3) | 0.0158 (7) |
| N2 | 0.3437 (5) | −0.2632 (3) | −0.1527 (2) | 0.0141 (6) |
| N3 | −0.1352 (5) | −0.5920 (3) | −0.1621 (3) | 0.0168 (7) |
| C1 | 0.5860 (6) | −0.1354 (3) | 0.1176 (3) | 0.0178 (8) |
| C2 | 0.4806 (5) | −0.1986 (3) | 0.0175 (3) | 0.0142 (8) |
| C3 | 0.4813 (5) | −0.1914 (3) | −0.0886 (3) | 0.0148 (8) |

| | | | | |
|---|---|---|---|---|
| C4 | 0.5922 (6) | −0.1201 (3) | −0.1406 (3) | 0.0172 (8) |
| C5 | 0.2647 (5) | −0.3130 (3) | −0.0826 (3) | 0.0144 (8) |
| C6 | 0.1198 (5) | −0.4054 (3) | −0.1148 (3) | 0.0151 (8) |
| C7 | −0.0568 (6) | −0.3944 (3) | −0.1030 (3) | 0.0161 (8) |
| H7 | −0.090 (7) | −0.323 (4) | −0.074 (4) | 0.029 (13)* |
| C8 | −0.1783 (6) | −0.4892 (4) | −0.1272 (3) | 0.0175 (8) |
| H8 | −0.297 (6) | −0.478 (4) | −0.122 (3) | 0.014 (10)* |
| C9 | 0.0311 (6) | −0.6007 (4) | −0.1785 (4) | 0.0231 (9) |
| H9 | 0.047 (6) | −0.676 (4) | −0.206 (4) | 0.023 (12)* |
| C10 | 0.1607 (6) | −0.5112 (4) | −0.1567 (3) | 0.0222 (9) |
| H10 | 0.285 (7) | −0.522 (4) | −0.161 (4) | 0.030 (13)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ni1 | 0.0168 (3) | 0.0167 (3) | 0.0120 (3) | −0.0020 (2) | 0.00689 (19) | −0.0009 (2) |
| O1 | 0.0247 (17) | 0.0394 (19) | 0.0202 (16) | −0.0164 (14) | 0.0058 (13) | −0.0018 (14) |
| O2 | 0.0272 (16) | 0.0310 (16) | 0.0141 (14) | −0.0091 (13) | 0.0097 (12) | −0.0055 (12) |
| O3 | 0.0250 (16) | 0.0351 (18) | 0.0218 (15) | −0.0181 (14) | 0.0068 (13) | 0.0018 (14) |
| O4 | 0.0247 (16) | 0.0259 (15) | 0.0155 (14) | −0.0076 (12) | 0.0107 (12) | 0.0026 (12) |
| O1W | 0.0235 (18) | 0.0257 (17) | 0.0274 (17) | 0.0037 (14) | 0.0134 (14) | 0.0046 (14) |
| N1 | 0.0180 (16) | 0.0177 (16) | 0.0133 (15) | −0.0024 (14) | 0.0074 (13) | 0.0009 (13) |
| N2 | 0.0172 (16) | 0.0152 (15) | 0.0126 (15) | −0.0023 (13) | 0.0085 (13) | 0.0000 (13) |
| N3 | 0.0197 (17) | 0.0187 (16) | 0.0124 (15) | −0.0032 (14) | 0.0059 (13) | 0.0012 (13) |
| C1 | 0.018 (2) | 0.021 (2) | 0.0136 (19) | −0.0036 (16) | 0.0045 (16) | 0.0010 (16) |
| C2 | 0.0104 (18) | 0.0183 (19) | 0.0136 (18) | −0.0043 (14) | 0.0034 (14) | −0.0016 (15) |
| C3 | 0.0158 (19) | 0.0160 (18) | 0.0151 (18) | −0.0024 (15) | 0.0087 (15) | 0.0015 (15) |
| C4 | 0.0165 (19) | 0.020 (2) | 0.018 (2) | −0.0020 (15) | 0.0091 (16) | 0.0035 (16) |
| C5 | 0.016 (2) | 0.0146 (18) | 0.0146 (18) | −0.0030 (15) | 0.0078 (15) | −0.0009 (15) |
| C6 | 0.017 (2) | 0.0199 (19) | 0.0086 (17) | −0.0038 (16) | 0.0054 (14) | 0.0005 (15) |
| C7 | 0.017 (2) | 0.0147 (19) | 0.0164 (19) | 0.0026 (15) | 0.0059 (15) | 0.0001 (16) |
| C8 | 0.014 (2) | 0.023 (2) | 0.0166 (19) | 0.0025 (16) | 0.0065 (15) | 0.0073 (16) |
| C9 | 0.028 (2) | 0.019 (2) | 0.027 (2) | −0.0057 (18) | 0.0151 (18) | −0.0062 (18) |
| C10 | 0.022 (2) | 0.026 (2) | 0.024 (2) | −0.0044 (17) | 0.0150 (18) | −0.0045 (18) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Ni1—O1W | 2.070 (3) | N2—C3 | 1.365 (5) |
| Ni1—N3$^{i}$ | 2.082 (3) | N2—Ni1$^{iii}$ | 2.105 (3) |
| Ni1—O4$^{ii}$ | 2.089 (3) | N3—C8 | 1.332 (5) |
| Ni1—O2 | 2.103 (3) | N3—C9 | 1.338 (5) |
| Ni1—N2$^{ii}$ | 2.105 (3) | N3—Ni1$^{i}$ | 2.082 (3) |
| Ni1—N1 | 2.134 (3) | C1—C2 | 1.465 (5) |
| O1—C1 | 1.299 (5) | C2—C3 | 1.372 (5) |
| O1—H1 | 0.94 (7) | C3—C4 | 1.474 (5) |
| O2—C1 | 1.230 (5) | C5—C6 | 1.474 (5) |
| O3—C4 | 1.285 (5) | C6—C7 | 1.390 (5) |
| O4—C4 | 1.246 (5) | C6—C10 | 1.396 (6) |

| | | | |
|---|---|---|---|
| O4—Ni1$^{iii}$ | 2.089 (3) | C7—C8 | 1.384 (6) |
| O1W—H1A | 0.78 (9) | C7—H7 | 0.96 (5) |
| O1W—H1B | 0.73 (6) | C8—H8 | 0.93 (4) |
| N1—C5 | 1.349 (5) | C9—C10 | 1.374 (6) |
| N1—C2 | 1.375 (5) | C9—H9 | 0.95 (5) |
| N2—C5 | 1.356 (5) | C10—H10 | 0.96 (5) |
| | | | |
| O1W—Ni1—N3$^{i}$ | 95.68 (14) | O2—C1—O1 | 122.1 (4) |
| O1W—Ni1—O4$^{ii}$ | 173.34 (13) | O2—C1—C2 | 119.2 (3) |
| N3$^{i}$—Ni1—O4$^{ii}$ | 89.89 (13) | O1—C1—C2 | 118.7 (3) |
| O1W—Ni1—O2 | 92.26 (14) | C3—C2—N1 | 109.0 (3) |
| N3$^{i}$—Ni1—O2 | 170.92 (13) | C3—C2—C1 | 132.3 (3) |
| O4$^{ii}$—Ni1—O2 | 82.49 (12) | N1—C2—C1 | 118.5 (3) |
| O1W—Ni1—N2$^{ii}$ | 94.71 (13) | N2—C3—C2 | 108.6 (3) |
| N3$^{i}$—Ni1—N2$^{ii}$ | 94.98 (12) | N2—C3—C4 | 118.9 (3) |
| O4$^{ii}$—Ni1—N2$^{ii}$ | 81.13 (11) | C2—C3—C4 | 132.4 (4) |
| O2—Ni1—N2$^{ii}$ | 88.74 (12) | O4—C4—O3 | 124.6 (4) |
| O1W—Ni1—N1 | 86.54 (13) | O4—C4—C3 | 118.2 (3) |
| N3$^{i}$—Ni1—N1 | 95.94 (12) | O3—C4—C3 | 117.1 (3) |
| O4$^{ii}$—Ni1—N1 | 96.54 (12) | N1—C5—N2 | 113.1 (3) |
| O2—Ni1—N1 | 80.11 (11) | N1—C5—C6 | 123.1 (3) |
| N2$^{ii}$—Ni1—N1 | 168.83 (12) | N2—C5—C6 | 123.7 (3) |
| C1—O1—H1 | 114 (4) | C7—C6—C10 | 117.3 (4) |
| C1—O2—Ni1 | 113.9 (3) | C7—C6—C5 | 123.2 (4) |
| C4—O4—Ni1$^{iii}$ | 113.4 (2) | C10—C6—C5 | 119.4 (3) |
| Ni1—O1W—H1A | 107 (6) | C8—C7—C6 | 119.2 (4) |
| Ni1—O1W—H1B | 130 (4) | C8—C7—H7 | 121 (3) |
| H1A—O1W—H1B | 107 (7) | C6—C7—H7 | 120 (3) |
| C5—N1—C2 | 104.4 (3) | N3—C8—C7 | 123.3 (4) |
| C5—N1—Ni1 | 146.9 (3) | N3—C8—H8 | 119 (3) |
| C2—N1—Ni1 | 108.0 (2) | C7—C8—H8 | 117 (3) |
| C5—N2—C3 | 104.9 (3) | N3—C9—C10 | 123.2 (4) |
| C5—N2—Ni1$^{iii}$ | 146.2 (3) | N3—C9—H9 | 111 (3) |
| C3—N2—Ni1$^{iii}$ | 108.1 (2) | C10—C9—H9 | 126 (3) |
| C8—N3—C9 | 117.5 (3) | C9—C10—C6 | 119.4 (4) |
| C8—N3—Ni1$^{i}$ | 119.6 (3) | C9—C10—H10 | 122 (3) |
| C9—N3—Ni1$^{i}$ | 122.9 (3) | C6—C10—H10 | 118 (3) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···O3 | 0.94 (7) | 1.57 (7) | 2.501 (4) | 171 (7) |
| O1*W*—H1*A*···O3$^{iv}$ | 0.78 (9) | 1.95 (9) | 2.726 (5) | 174 (9) |
| O1*W*—H1*B*···O1$^{v}$ | 0.73 (6) | 2.35 (6) | 3.007 (5) | 150 (5) |

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