Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# *catena*-Poly[[[diaquadiformatonickel(II)]-*μ*-1,4-bis(1*H*-benzimidazol-1-yl)benzene] dihydrate]

**Hui Li,* Hong Sun, Xiaochuan Chai and Chenzhong Yao**

Department of Applied Chemistry, Yuncheng University, Yuncheng, Shanxi 044000, People's Republic of China
Correspondence e-mail: lihuiwff@163.com

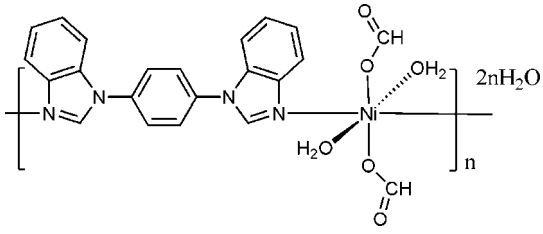
Received 13 January 2012; accepted 23 January 2012

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.027; $wR$ factor = 0.061; data-to-parameter ratio = 12.5.

In the title one-dimensional coordination polymer, $\{[Ni(CHO_2)_2(C_{20}H_{14}N_4)(H_2O)_2]\cdot 2H_2O\}_n$, the $Ni^{II}$ atom lies on a crystallographic inversion centre. It is coordinated by two formate O atoms, two water O atoms and two N atoms from two 1,4-bis(1*H*-benzimidazol-1-yl)benzene (bzb) ligands, resulting in a distorted *trans*-$NiN_2O_4$ octahedral coordination geometry. The bzb molecule acts as a bridging ligand to connect the metal atoms into a chain propagating in [1$\bar{1}\bar{1}$]. The dihedral angle between the benzimidazole ring and the central benzene ring in the ligand is 38.16 (9)°. In the crystal, O—H···O hydrogen bonds crosslink the chains into (010) sheets.

## Related literature

For background to coordination polymers containing imidazole-derived ligands, see: Li *et al.* (2009, 2011).




## Experimental

### Crystal data

$[Ni(CHO_2)_2(C_{20}H_{14}N_4)(H_2O)_2]\cdot 2H_2O$
$M_r$ = 531.16
Triclinic, $P\bar{1}$
$a$ = 7.4431 (15) Å
$b$ = 9.0895 (18) Å
$c$ = 9.3863 (19) Å
$\alpha$ = 78.46 (3)°
$\beta$ = 77.79 (3)°
$\gamma$ = 67.86 (3)°
$V$ = 569.8 (2) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 0.91 mm$^{-1}$
$T$ = 293 K
0.25 × 0.22 × 0.20 mm

### Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min}$ = 0.797, $T_{max}$ = 0.834
5022 measured reflections
2000 independent reflections
1874 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.061
$S$ = 1.09
2000 reflections
160 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Ni1—O1 | 2.0695 (14) | Ni1—O1*W* | 2.1036 (16) |
| Ni1—N1 | 2.0908 (16) | | |

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*A*···O2$^{i}$ | 0.85 | 1.85 | 2.694 (2) | 169 |
| O1*W*—H1*B*···O2*W*$^{ii}$ | 0.85 | 1.92 | 2.762 (2) | 169 |
| O2*W*—H2*A*···O2$^{iii}$ | 0.85 | 1.91 | 2.760 (2) | 173 |
| O2*W*—H2*B*···O1$^{iv}$ | 0.85 | 2.16 | 2.846 (2) | 137 |

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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 authors thank the Young Scientist Fund of the NSFC of China (grant No. 51101138) and the College Research Program of Yuncheng University (grant No. 2008114) for funding.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6604).

## References

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# supporting information

*Acta Cryst.* (2012). E**68**, m216 [doi:10.1107/S160053681200284X]

## *catena*-Poly[[[diaquadiformatonickel(II)]-$\mu$-1,4-bis(1*H*-benzimidazol-1-yl)benzene] dihydrate]

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### S1. Comment

Imidazole has been extensively used in crystal engineering, and a large number of imidazole-containing flexible ligands have been extensively studied. However, to our knowledge, the research on imidazole ligands bearing rigid spacers is still less developed (Li *et al.*, 2009; Li *et al.*, 2011). For the title compound, the geometry of the $Ni^{II}$ ion is bound by two benzimidazole rings of individual **L** ligands, two water molecules and two formate ions forming a slightly distorted octahedral coordination environment(Fig. 1). Notably, as shown in Fig. 2, the six-coordinate $Ni^{II}$ center is bridged by the ligand **L** to form an infinite one-dimensional architecture.

### S2. Experimental

A mixture of $CH_3OH$ and $H_2O$ (1:1, 8 ml), as a buffer layer, was carefully layered over a solution of $Ni(HCO_2)_2$ in $H_2O$ (6 ml). Then a solution of 1,4-di(1*H*-benzimidazol-1-yl)benzene (**L**, 0.06 mmol) in $CH_3OH$ (6 ml) was layered over the buffer layer, and the resultant reaction was left to stand at room temperature. After *ca* three weeks, green block single crystals appeared at the boundary. Yield: ~20% (based on **L**).

### S3. Refinement

C-bound H atoms were positioned geometrically and refined in the riding-model approximation, with C—H = 0.93Å and $U_{iso}$(H) = 1.2$U_{eq}$ (C).

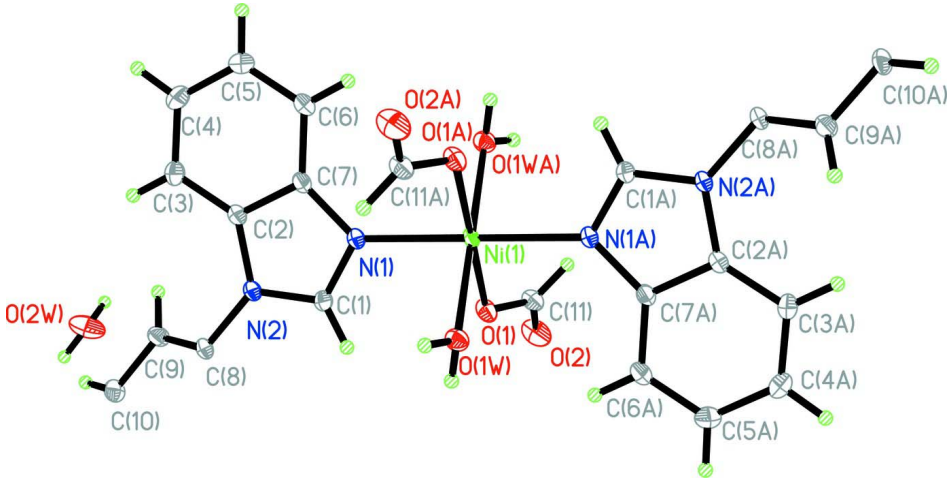


**Figure 1**

The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius.

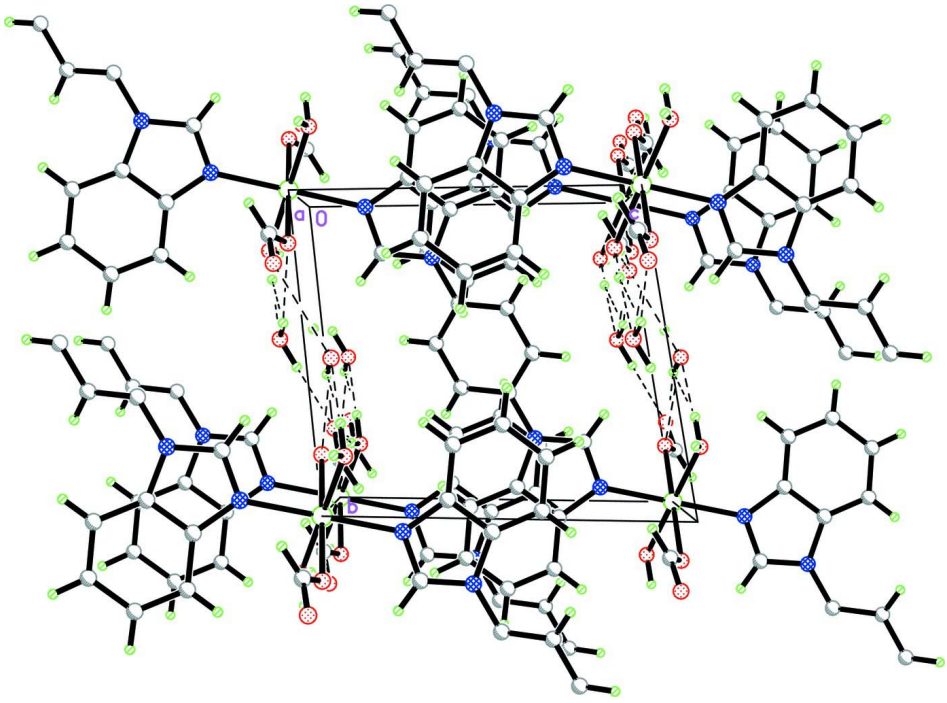

**Figure 2**

The crystal packing for (**I**).

***catena*-Poly[[[diaquadiformatonickel(II)]-*μ*-1,4- bis(1*H*-benzimidazol-1-yl)benzene] dihydrate]**

*Crystal data*

$[Ni(CHO_2)_2(C_{20}H_{14}N_4)(H_2O)_2]\cdot 2H_2O$
$M_r = 531.16$
Triclinic, $P\overline{1}$
Hall symbol: -p 1
$a = 7.4431\ (15)$ Å
$b = 9.0895\ (18)$ Å
$c = 9.3863\ (19)$ Å
$\alpha = 78.46\ (3)°$
$\beta = 77.79\ (3)°$
$\gamma = 67.86\ (3)°$
$V = 569.8\ (2)$ Å$^3$
$Z = 1$
$F(000) = 276$
$D_x = 1.548$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6111 reflections
$\theta = 6.2–55.0°$
$\mu = 0.91$ mm$^{-1}$
$T = 293$ K
Block, green
0.25 × 0.22 × 0.20 mm

*Data collection*

Rigaku Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.797$, $T_{max} = 0.834$
5022 measured reflections
2000 independent reflections
1874 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.1°$
$h = -8\rightarrow 8$
$k = -10\rightarrow 10$
$l = -11\rightarrow 11$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.061$
$S = 1.09$
2000 reflections
160 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0208P)^2 + 0.3422P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å$^{-3}$
$\Delta\rho_{min} = -0.19$ 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 | 0.0000 | 0.0000 | 0.01789 (11) |
| N1 | 0.8599 (2) | 0.05059 (18) | 0.21160 (16) | 0.0233 (4) |
| N2 | 0.7076 (2) | 0.21017 (19) | 0.38522 (17) | 0.0251 (4) |
| O1 | 1.11753 (19) | 0.17566 (16) | −0.00983 (15) | 0.0272 (3) |
| O2 | 1.3775 (2) | 0.24681 (19) | −0.03883 (19) | 0.0439 (4) |
| O2W | 0.8143 (3) | 0.4708 (2) | 0.9185 (2) | 0.0580 (5) |
| O1W | 0.76721 (19) | 0.18582 (16) | −0.09086 (15) | 0.0265 (3) |
| C1 | 0.7822 (3) | 0.1980 (2) | 0.2416 (2) | 0.0265 (4) |
| H1 | 0.7785 | 0.2864 | 0.1709 | 0.032* |
| C2 | 0.7415 (3) | 0.0544 (2) | 0.4562 (2) | 0.0243 (4) |
| C3 | 0.6960 (3) | −0.0069 (3) | 0.6010 (2) | 0.0349 (5) |
| H3 | 0.6319 | 0.0598 | 0.6733 | 0.042* |
| C4 | 0.7496 (4) | −0.1702 (3) | 0.6330 (2) | 0.0410 (6) |
| H4 | 0.7235 | −0.2156 | 0.7294 | 0.049* |
| C5 | 0.8426 (3) | −0.2698 (3) | 0.5238 (3) | 0.0390 (5) |
| H5 | 0.8762 | −0.3800 | 0.5493 | 0.047* |
| C6 | 0.8858 (3) | −0.2091 (2) | 0.3798 (2) | 0.0301 (5) |
| H6 | 0.9465 | −0.2762 | 0.3076 | 0.036* |
| C7 | 0.8359 (3) | −0.0440 (2) | 0.3458 (2) | 0.0223 (4) |
| C8 | 0.6026 (3) | 0.3572 (2) | 0.4442 (2) | 0.0242 (4) |
| C9 | 0.6216 (3) | 0.3723 (2) | 0.5828 (2) | 0.0280 (5) |
| H9 | 0.7031 | 0.2864 | 0.6386 | 0.034* |
| C10 | 0.5193 (3) | 0.5154 (2) | 0.6388 (2) | 0.0292 (5) |
| H10 | 0.5321 | 0.5262 | 0.7322 | 0.035* |
| C11 | 1.2948 (3) | 0.1551 (2) | −0.0493 (2) | 0.0280 (5) |

| | | | | |
|---|---|---|---|---|
| H11 | 1.3723 | 0.0622 | −0.0905 | 0.034* |
| H1A | 0.6479 | 0.1921 | −0.0709 | 0.042* |
| H1B | 0.7658 | 0.2799 | −0.0905 | 0.042* |
| H2A | 0.7644 | 0.5582 | 0.9559 | 0.042* |
| H2B | 0.9293 | 0.4212 | 0.9405 | 0.042* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ni1 | 0.01748 (19) | 0.01802 (19) | 0.01746 (19) | −0.00478 (14) | 0.00105 (13) | −0.00749 (13) |
| N1 | 0.0272 (9) | 0.0210 (9) | 0.0184 (8) | −0.0052 (7) | 0.0011 (7) | −0.0064 (7) |
| N2 | 0.0323 (9) | 0.0199 (8) | 0.0185 (8) | −0.0045 (7) | 0.0018 (7) | −0.0073 (6) |
| O1 | 0.0218 (7) | 0.0261 (8) | 0.0348 (8) | −0.0090 (6) | 0.0019 (6) | −0.0117 (6) |
| O2 | 0.0276 (8) | 0.0366 (9) | 0.0723 (12) | −0.0153 (7) | −0.0012 (8) | −0.0161 (8) |
| O2W | 0.0580 (12) | 0.0302 (9) | 0.0900 (15) | −0.0068 (8) | −0.0309 (10) | −0.0132 (9) |
| O1W | 0.0220 (7) | 0.0249 (7) | 0.0311 (8) | −0.0061 (6) | −0.0041 (6) | −0.0041 (6) |
| C1 | 0.0348 (11) | 0.0218 (10) | 0.0185 (10) | −0.0068 (9) | 0.0017 (8) | −0.0052 (8) |
| C2 | 0.0247 (10) | 0.0217 (10) | 0.0230 (10) | −0.0043 (8) | 0.0000 (8) | −0.0067 (8) |
| C3 | 0.0440 (13) | 0.0329 (12) | 0.0215 (11) | −0.0100 (10) | 0.0042 (9) | −0.0063 (9) |
| C4 | 0.0539 (15) | 0.0345 (13) | 0.0257 (12) | −0.0133 (11) | 0.0021 (10) | 0.0031 (9) |
| C5 | 0.0459 (14) | 0.0235 (11) | 0.0397 (13) | −0.0089 (10) | 0.0003 (10) | 0.0002 (9) |
| C6 | 0.0308 (11) | 0.0234 (11) | 0.0311 (12) | −0.0045 (9) | 0.0016 (9) | −0.0091 (9) |
| C7 | 0.0209 (10) | 0.0218 (10) | 0.0221 (10) | −0.0044 (8) | −0.0010 (8) | −0.0068 (8) |
| C8 | 0.0267 (10) | 0.0217 (10) | 0.0207 (10) | −0.0047 (8) | 0.0021 (8) | −0.0087 (8) |
| C9 | 0.0321 (11) | 0.0234 (10) | 0.0238 (11) | −0.0020 (9) | −0.0065 (8) | −0.0059 (8) |
| C10 | 0.0378 (12) | 0.0290 (11) | 0.0186 (10) | −0.0061 (9) | −0.0038 (8) | −0.0097 (8) |
| C11 | 0.0241 (11) | 0.0248 (11) | 0.0333 (12) | −0.0057 (9) | −0.0026 (9) | −0.0075 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Ni1—O1$^{i}$ | 2.0695 (14) | C2—C3 | 1.385 (3) |
| Ni1—O1 | 2.0695 (14) | C2—C7 | 1.399 (3) |
| Ni1—N1$^{i}$ | 2.0908 (16) | C3—C4 | 1.371 (3) |
| Ni1—N1 | 2.0908 (16) | C3—H3 | 0.9300 |
| Ni1—O1W | 2.1036 (16) | C4—C5 | 1.395 (3) |
| Ni1—O1W$^{i}$ | 2.1036 (16) | C4—H4 | 0.9300 |
| N1—C1 | 1.307 (2) | C5—C6 | 1.373 (3) |
| N1—C7 | 1.395 (2) | C5—H5 | 0.9300 |
| N2—C1 | 1.354 (2) | C6—C7 | 1.389 (3) |
| N2—C2 | 1.391 (2) | C6—H6 | 0.9300 |
| N2—C8 | 1.424 (2) | C8—C9 | 1.377 (3) |
| O1—C11 | 1.245 (2) | C8—C10$^{ii}$ | 1.385 (3) |
| O2—C11 | 1.236 (2) | C9—C10 | 1.380 (3) |
| O2W—H2A | 0.8522 | C9—H9 | 0.9300 |
| O2W—H2B | 0.8516 | C10—C8$^{ii}$ | 1.385 (3) |
| O1W—H1A | 0.8504 | C10—H10 | 0.9300 |
| O1W—H1B | 0.8516 | C11—H11 | 0.9300 |
| C1—H1 | 0.9300 | | |

| | | | |
|---|---|---|---|
| O1$^{i}$—Ni1—O1 | 180.00 (5) | C3—C2—C7 | 122.24 (18) |
| O1$^{i}$—Ni1—N1$^{i}$ | 87.66 (6) | N2—C2—C7 | 105.25 (16) |
| O1—Ni1—N1$^{i}$ | 92.34 (6) | C4—C3—C2 | 116.98 (19) |
| O1$^{i}$—Ni1—N1 | 92.34 (6) | C4—C3—H3 | 121.5 |
| O1—Ni1—N1 | 87.66 (6) | C2—C3—H3 | 121.5 |
| N1$^{i}$—Ni1—N1 | 180.00 (10) | C3—C4—C5 | 121.4 (2) |
| O1$^{i}$—Ni1—O1W | 94.56 (6) | C3—C4—H4 | 119.3 |
| O1—Ni1—O1W | 85.44 (6) | C5—C4—H4 | 119.3 |
| N1$^{i}$—Ni1—O1W | 89.72 (6) | C6—C5—C4 | 121.7 (2) |
| N1—Ni1—O1W | 90.28 (6) | C6—C5—H5 | 119.2 |
| O1$^{i}$—Ni1—O1W$^{i}$ | 85.44 (6) | C4—C5—H5 | 119.2 |
| O1—Ni1—O1W$^{i}$ | 94.56 (6) | C5—C6—C7 | 117.75 (19) |
| N1$^{i}$—Ni1—O1W$^{i}$ | 90.28 (6) | C5—C6—H6 | 121.1 |
| N1—Ni1—O1W$^{i}$ | 89.72 (6) | C7—C6—H6 | 121.1 |
| O1W—Ni1—O1W$^{i}$ | 180.00 (11) | C6—C7—N1 | 130.60 (17) |
| C1—N1—C7 | 105.03 (15) | C6—C7—C2 | 119.93 (18) |
| C1—N1—Ni1 | 120.95 (13) | N1—C7—C2 | 109.45 (16) |
| C7—N1—Ni1 | 133.87 (12) | C9—C8—C10$^{ii}$ | 120.26 (18) |
| C1—N2—C2 | 106.47 (16) | C9—C8—N2 | 120.29 (18) |
| C1—N2—C8 | 124.79 (17) | C10$^{ii}$—C8—N2 | 119.45 (17) |
| C2—N2—C8 | 128.57 (16) | C8—C9—C10 | 119.76 (19) |
| C11—O1—Ni1 | 123.29 (13) | C8—C9—H9 | 120.1 |
| H2A—O2W—H2B | 109.0 | C10—C9—H9 | 120.1 |
| Ni1—O1W—H1A | 124.7 | C9—C10—C8$^{ii}$ | 119.98 (18) |
| Ni1—O1W—H1B | 114.7 | C9—C10—H10 | 120.0 |
| H1A—O1W—H1B | 105.8 | C8$^{ii}$—C10—H10 | 120.0 |
| N1—C1—N2 | 113.79 (18) | O2—C11—O1 | 126.04 (19) |
| N1—C1—H1 | 123.1 | O2—C11—H11 | 117.0 |
| N2—C1—H1 | 123.1 | O1—C11—H11 | 117.0 |
| C3—C2—N2 | 132.49 (18) | | |

| | | | |
|---|---|---|---|
| O1$^{i}$—Ni1—N1—C1 | −139.94 (16) | N2—C2—C3—C4 | 178.9 (2) |
| O1—Ni1—N1—C1 | 40.06 (16) | C7—C2—C3—C4 | 0.7 (3) |
| N1$^{i}$—Ni1—N1—C1 | 152 (100) | C2—C3—C4—C5 | −1.2 (4) |
| O1W—Ni1—N1—C1 | −45.36 (16) | C3—C4—C5—C6 | 0.4 (4) |
| O1W$^{i}$—Ni1—N1—C1 | 134.64 (16) | C4—C5—C6—C7 | 0.8 (3) |
| O1$^{i}$—Ni1—N1—C7 | 45.25 (18) | C5—C6—C7—N1 | −179.6 (2) |
| O1—Ni1—N1—C7 | −134.75 (18) | C5—C6—C7—C2 | −1.2 (3) |
| N1$^{i}$—Ni1—N1—C7 | −23 (100) | C1—N1—C7—C6 | 178.2 (2) |
| O1W—Ni1—N1—C7 | 139.83 (18) | Ni1—N1—C7—C6 | −6.4 (3) |
| O1W$^{i}$—Ni1—N1—C7 | −40.17 (18) | C1—N1—C7—C2 | −0.3 (2) |
| O1$^{i}$—Ni1—O1—C11 | 90 (100) | Ni1—N1—C7—C2 | 175.08 (14) |
| N1$^{i}$—Ni1—O1—C11 | −48.98 (16) | C3—C2—C7—C6 | 0.5 (3) |
| N1—Ni1—O1—C11 | 131.02 (16) | N2—C2—C7—C6 | −178.12 (18) |
| O1W—Ni1—O1—C11 | −138.51 (16) | C3—C2—C7—N1 | 179.16 (19) |
| O1W$^{i}$—Ni1—O1—C11 | 41.49 (16) | N2—C2—C7—N1 | 0.6 (2) |
| C7—N1—C1—N2 | −0.1 (2) | C1—N2—C8—C9 | −145.1 (2) |

| | | | |
|---|---|---|---|
| Ni1—N1—C1—N2 | −176.23 (13) | C2—N2—C8—C9 | 40.3 (3) |
| C2—N2—C1—N1 | 0.5 (2) | C1—N2—C8—C10$^{ii}$ | 35.2 (3) |
| C8—N2—C1—N1 | −175.17 (18) | C2—N2—C8—C10$^{ii}$ | −139.5 (2) |
| C1—N2—C2—C3 | −179.0 (2) | C10$^{ii}$—C8—C9—C10 | −0.3 (3) |
| C8—N2—C2—C3 | −3.6 (4) | N2—C8—C9—C10 | 179.95 (18) |
| C1—N2—C2—C7 | −0.6 (2) | C8—C9—C10—C8$^{ii}$ | 0.3 (3) |
| C8—N2—C2—C7 | 174.80 (18) | Ni1—O1—C11—O2 | −169.69 (16) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*A*···O2$^{iii}$ | 0.85 | 1.85 | 2.694 (2) | 169 |
| O1*W*—H1*B*···O2*W*$^{iv}$ | 0.85 | 1.92 | 2.762 (2) | 169 |
| O2*W*—H2*A*···O2$^{v}$ | 0.85 | 1.91 | 2.760 (2) | 173 |
| O2*W*—H2*B*···O1$^{vi}$ | 0.85 | 2.16 | 2.846 (2) | 137 |

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