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# Tetraaqua(2,2′-bipyridine-$\kappa^2N,N'$)-nickel(II) cyclohexane-1,4-dicarboxylate

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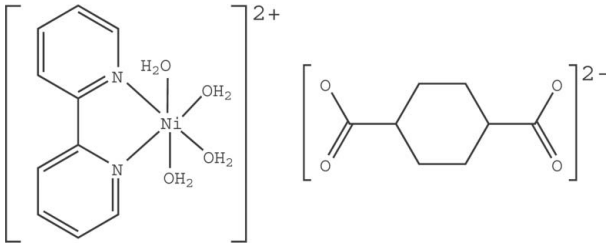
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.009 Å; disorder in solvent or counterion; $R$ factor = 0.049; $wR$ factor = 0.130; data-to-parameter ratio = 14.0.

In the title compound, $[Ni(C_{10}H_8N_2)(H_2O)_4](C_8H_{10}O_4)$, the $Ni^{II}$ ion is located on a twofold rotation axis and has a distorted octahedral geometry formed by a chelating 2,2′-bipyridine ligand and four water molecules. The disordered cyclohexane-1,4-dicarboxylate dianion is located across another twofold rotation axis and adopts a boat conformation. O—H···O hydrogen bonding between the complex cation and the cyclohexane-1,4-dicarboxylate dianion helps to stabilize the crystal structure.

## Related literature

For related metal complexes with the cyclohexane-1,4-dicarboxylate ligand, see: Kurmoo *et al.* (2006, 2003); Qi *et al.* (2003); Rao *et al.* (2007); Yu *et al.* (2006, 2007).




## Experimental

### Crystal data

$[Ni(C_{10}H_8N_2)(H_2O)_4](C_8H_{10}O_4)$
$M_r$ = 457.12
Monoclinic, $C2/c$
$a$ = 11.9151 (16) Å
$b$ = 24.642 (4) Å
$c$ = 7.5556 (9) Å
$\beta$ = 115.313 (2)°
$V$ = 2005.4 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.02 mm$^{-1}$
$T$ = 298 (2) K
0.28 × 0.27 × 0.26 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan *SADABS* (Bruker, 1997)
$T_{min}$ = 0.762, $T_{max}$ = 0.771
5087 measured reflections
1811 independent reflections
1619 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.130
$S$ = 1.04
1811 reflections
129 parameters
8 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.81 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.60 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$W$···O2$^{i}$ | 0.81 | 2.00 | 2.759 (4) | 157 |
| O1$W$—H2$W$···O2$^{ii}$ | 0.81 | 1.83 | 2.637 (4) | 175 |
| O2$W$—H3$W$···O1 | 0.92 | 1.87 | 2.754 (4) | 162 |
| O2$W$—H4$W$···O1$^{iii}$ | 0.89 | 1.79 | 2.678 (4) | 173 |

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *DIAMOND* (Brandenburg, 1998); 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: XU2285).

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# supplementary materials

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# Tetraaqua(2,2'-bipyridine-$\kappa^2N,N'$)nickel(II) cyclohexane-1,4-dicarboxylate

**M. Yu, S.-X. Liu, L.-H. Xie, R.-G. Cao and Y.-H. Ren**

## Comment

Cyclohexane-1,4-dicarboxylic acid ($H_2$chdc) is a flexible ligand for constructing functional metal-organic frameworks (Qi *et al.*, 2003; Kurmoo *et al.*, 2003, 2006; Rao *et al.*, 2007). As part of investigation on cyclohexane-1,4-dicarboxylate complexes (Yu *et al.*, 2006, 2007), we present here the crystal structure of the title $Ni^{II}$ complex.

The crystal of the $Ni^{II}$ compound consists of $[Ni(2,2'\text{-bpy})(H_2O)_4]^{2+}$ cations and cyclohexane-1,4-dicarboxylate dianions. The complex cation and conter-dianion are located on individual twofold rotation axis. In the cation, Ni atom coordinates with two N atoms from a 2,2'-bpy ligand and four water molecules in a distorted octahedral geometry (Figure 1). The chdc anion is disordered and it has been modeled at two positions with their occupancies set to be 0.5. Hydrogen bonding (Table 1) between coordinated water molecules of the complex cations and carboxyl O atoms of chdc anions results in a double layer supra-molecular structure along *ac* plane (Figure 2, Figure 3).

## Experimental

$NiCl_2{\cdot}6H_2O$ (0.6 mmol, 0.143 g) and $H_2$chdc (0.6 mmol, 0.103 g) were dissolved in 18 ml water. Then an ethanol solution (8 ml) of 2,2'-bipyridine (0.6 mmol, 0.094 g) was mixed with the solution. The pH value of the solution was adjusted to 7.0 with diluted NaOH solution. The mixture was then refluxed at 363 K for 12 h. The filtrate was kept under room temperature for about two weeks. Single crystals of the title compound were obtained from the filtrate yield.

## Refinement

H atoms on water molecules were located in a difference Fourier map and refined as ringing in their as-found relative positions, $U_{iso}(H) = 1.5U_{eq}(O)$. The others H atoms were placed in calculated positions and refined in the riding model approximation with C—H = 0.93 or 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The cyclohexane ring of chdc anion is disordered, and the disorder was modeled as two components. The occupancies of both components were set to be 1/2, and the geometries of the two components were restrained with C—C = 1.54 Å. The displacement parameters of C atoms of the disordered cyclohexane ring were restrained to be equal.

## Figures

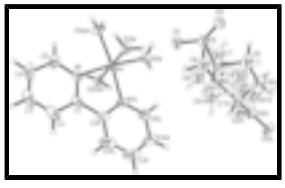

Fig. 1. The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level. The chdc anion is disordered at two positions with one part shown with open bonds.

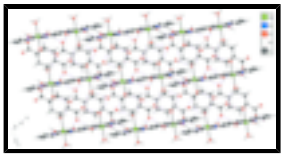

Fig. 2. Perspective view of the two-dimensional double layer along *b* axis. Hydrogen bonds are represented by pink dashed lines.

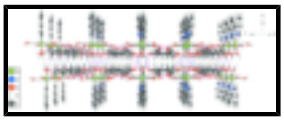

Fig. 3. Side view of the double layer.

## Tetraaqua(2,2'-bipyridine-κ$^2$*N*,*N*')nickel(II) cyclohexane-1,4-dicarboxylate

*Crystal data*

| | |
|---|---|
| $[Ni(C_{10}H_8N_2)(H_2O)_4](C_8H_{10}O_4)$ | $F_{000}$ = 960 |
| $M_r$ = 457.12 | $D_x$ = 1.514 Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 2378 reflections |
| *a* = 11.9151 (16) Å | θ = 1.6–25.0º |
| *b* = 24.642 (4) Å | μ = 1.02 mm$^{-1}$ |
| *c* = 7.5556 (9) Å | *T* = 298 (2) K |
| β = 115.313 (2)º | Block, green |
| *V* = 2005.4 (5) Å$^3$ | 0.28 × 0.27 × 0.26 mm |
| *Z* = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 1811 independent reflections |
| Radiation source: fine-focus sealed tube | 1619 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.024 |
| *T* = 298(2) K | $\theta_{max}$ = 25.2º |
| φ and ω scans | $\theta_{min}$ = 1.6º |
| Absorption correction: multi-scan SADABS (Bruker, 1997) | *h* = −14→11 |
| $T_{min}$ = 0.762, $T_{max}$ = 0.771 | *k* = −29→29 |
| 5087 measured reflections | *l* = −3→9 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.049 | H-atom parameters constrained |
| $wR(F^2)$ = 0.130 | $w = 1/[\sigma^2(F_o^2) + (0.0627P)^2 + 7.6283P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| *S* = 1.04 | $(\Delta/\sigma)_{max} < 0.001$ |

| | |
|---|---|
| 1811 reflections | $\Delta\rho_{max}$ = 0.81 e Å$^{-3}$ |
| 129 parameters | $\Delta\rho_{min}$ = −0.60 e Å$^{-3}$ |
| 8 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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Ni1 | 0.5000 | 0.35801 (2) | 0.2500 | 0.0293 (2) | |
| O1W | 0.3653 (3) | 0.30106 (12) | 0.1394 (4) | 0.0564 (8) | |
| H1W | 0.3677 | 0.2717 | 0.1897 | 0.085* | |
| H2W | 0.3167 | 0.3006 | 0.0243 | 0.085* | |
| O2W | 0.4852 (2) | 0.35990 (11) | 0.5128 (4) | 0.0464 (7) | |
| H3W | 0.4164 | 0.3521 | 0.5339 | 0.070* | |
| H4W | 0.5565 | 0.3538 | 0.6170 | 0.070* | |
| N1 | 0.6216 (3) | 0.42334 (13) | 0.3502 (4) | 0.0414 (7) | |
| C1 | 0.5681 (4) | 0.47248 (16) | 0.3031 (6) | 0.0492 (10) | |
| C2 | 0.6395 (6) | 0.5193 (2) | 0.3525 (9) | 0.0786 (16) | |
| H2 | 0.6013 | 0.5531 | 0.3180 | 0.094* | |
| C3 | 0.7648 (7) | 0.5161 (3) | 0.4509 (10) | 0.097 (2) | |
| H3 | 0.8130 | 0.5474 | 0.4839 | 0.117* | |
| C4 | 0.8184 (5) | 0.4668 (3) | 0.5002 (9) | 0.0854 (18) | |
| H4 | 0.9042 | 0.4638 | 0.5679 | 0.102* | |
| C5 | 0.7448 (4) | 0.4204 (2) | 0.4495 (6) | 0.0585 (11) | |
| H5 | 0.7823 | 0.3866 | 0.4855 | 0.070* | |
| C6 | 0.2126 (3) | 0.32072 (17) | 0.6345 (5) | 0.0441 (9) | |
| O1 | 0.3097 (2) | 0.34452 (14) | 0.6550 (4) | 0.0558 (8) | |
| O2 | 0.1963 (3) | 0.30016 (12) | 0.7729 (4) | 0.0537 (8) | |
| C7 | 0.0998 (5) | 0.3329 (4) | 0.4395 (8) | 0.0738 (19) | 0.50 |
| H7 | 0.0849 | 0.3720 | 0.4190 | 0.089* | 0.50 |
| C8 | 0.1280 (8) | 0.3070 (5) | 0.2776 (10) | 0.0738 (19) | 0.50 |
| H8A | 0.1610 | 0.2709 | 0.3196 | 0.089* | 0.50 |
| H8B | 0.1924 | 0.3282 | 0.2636 | 0.089* | 0.50 |
| C9 | −0.0169 (7) | 0.3026 (6) | 0.4245 (12) | 0.0738 (19) | 0.50 |
| H9A | 0.0035 | 0.2646 | 0.4540 | 0.089* | 0.50 |

| | | | | | |
|---|---|---|---|---|---|
| H9B | −0.0411 | 0.3169 | 0.5227 | 0.089* | 0.50 |
| C7' | 0.1074 (6) | 0.3070 (4) | 0.4328 (7) | 0.0738 (19) | 0.50 |
| H7' | 0.0935 | 0.2679 | 0.4108 | 0.089* | 0.50 |
| C8' | 0.1261 (8) | 0.3360 (5) | 0.2670 (11) | 0.0738 (19) | 0.50 |
| H8'1 | 0.1909 | 0.3175 | 0.2450 | 0.089* | 0.50 |
| H8'2 | 0.1537 | 0.3729 | 0.3074 | 0.089* | 0.50 |
| C9' | −0.0073 (7) | 0.3375 (5) | 0.4261 (12) | 0.0738 (19) | 0.50 |
| H9'1 | −0.0272 | 0.3229 | 0.5285 | 0.089* | 0.50 |
| H9'2 | 0.0157 | 0.3752 | 0.4582 | 0.089* | 0.50 |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ni1 | 0.0283 (3) | 0.0319 (3) | 0.0221 (3) | 0.000 | 0.0055 (2) | 0.000 |
| O1W | 0.0597 (17) | 0.0521 (16) | 0.0330 (14) | −0.0236 (14) | −0.0035 (13) | 0.0093 (12) |
| O2W | 0.0352 (13) | 0.0742 (19) | 0.0267 (13) | 0.0003 (12) | 0.0104 (11) | 0.0033 (12) |
| N1 | 0.0452 (18) | 0.0455 (18) | 0.0326 (16) | −0.0096 (14) | 0.0157 (14) | −0.0065 (13) |
| C1 | 0.075 (3) | 0.038 (2) | 0.042 (2) | −0.0087 (19) | 0.032 (2) | −0.0033 (16) |
| C2 | 0.113 (5) | 0.046 (3) | 0.087 (4) | −0.023 (3) | 0.052 (4) | −0.012 (3) |
| C3 | 0.111 (5) | 0.075 (4) | 0.106 (5) | −0.057 (4) | 0.046 (4) | −0.030 (4) |
| C4 | 0.064 (3) | 0.109 (5) | 0.074 (4) | −0.044 (3) | 0.022 (3) | −0.024 (3) |
| C5 | 0.045 (2) | 0.076 (3) | 0.049 (2) | −0.016 (2) | 0.0145 (19) | −0.012 (2) |
| C6 | 0.0335 (19) | 0.059 (2) | 0.0286 (19) | −0.0039 (17) | 0.0026 (15) | 0.0038 (16) |
| O1 | 0.0368 (15) | 0.090 (2) | 0.0324 (14) | −0.0174 (14) | 0.0067 (12) | 0.0066 (14) |
| O2 | 0.0452 (15) | 0.0683 (19) | 0.0330 (14) | −0.0215 (14) | 0.0028 (12) | 0.0082 (13) |
| C7 | 0.0413 (16) | 0.130 (6) | 0.0346 (16) | −0.009 (3) | 0.0013 (14) | 0.011 (2) |
| C8 | 0.0413 (16) | 0.130 (6) | 0.0346 (16) | −0.009 (3) | 0.0013 (14) | 0.011 (2) |
| C9 | 0.0413 (16) | 0.130 (6) | 0.0346 (16) | −0.009 (3) | 0.0013 (14) | 0.011 (2) |
| C7' | 0.0413 (16) | 0.130 (6) | 0.0346 (16) | −0.009 (3) | 0.0013 (14) | 0.011 (2) |
| C8' | 0.0413 (16) | 0.130 (6) | 0.0346 (16) | −0.009 (3) | 0.0013 (14) | 0.011 (2) |
| C9' | 0.0413 (16) | 0.130 (6) | 0.0346 (16) | −0.009 (3) | 0.0013 (14) | 0.011 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Ni1—O1W | 2.024 (3) | C6—O2 | 1.250 (5) |
| Ni1—O1W$^{i}$ | 2.024 (3) | C6—C7' | 1.540 (2) |
| Ni1—O2W$^{i}$ | 2.068 (3) | C6—C7 | 1.540 (2) |
| Ni1—O2W | 2.068 (3) | C7—C8 | 1.538 (2) |
| Ni1—N1 | 2.080 (3) | C7—C9 | 1.540 (2) |
| Ni1—N1$^{i}$ | 2.080 (3) | C7—H7 | 0.9800 |
| O1W—H1W | 0.8112 | C8—C9$^{ii}$ | 1.539 (2) |
| O1W—H2W | 0.8133 | C8—H8A | 0.9700 |
| O2W—H3W | 0.9183 | C8—H8B | 0.9700 |
| O2W—H4W | 0.8902 | C9—C8$^{ii}$ | 1.539 (2) |
| N1—C5 | 1.335 (5) | C9—H9A | 0.9700 |
| N1—C1 | 1.344 (5) | C9—H9B | 0.9700 |
| C1—C2 | 1.388 (6) | C7'—C8' | 1.538 (2) |

| | | | |
|---|---|---|---|
| C1—C1$^{i}$ | 1.471 (9) | C7'—C9' | 1.541 (2) |
| C2—C3 | 1.355 (9) | C7'—H7' | 0.9800 |
| C2—H2 | 0.9300 | C8'—C9'$^{ii}$ | 1.539 (2) |
| C3—C4 | 1.350 (9) | C8'—H8'1 | 0.9700 |
| C3—H3 | 0.9300 | C8'—H8'2 | 0.9700 |
| C4—C5 | 1.391 (7) | C9'—C8'$^{ii}$ | 1.539 (2) |
| C4—H4 | 0.9300 | C9'—H9'1 | 0.9700 |
| C5—H5 | 0.9300 | C9'—H9'2 | 0.9700 |
| C6—O1 | 1.247 (5) | | |
| O1W—Ni1—O1W$^{i}$ | 92.22 (18) | O1—C6—C7' | 123.1 (4) |
| O1W—Ni1—O2W$^{i}$ | 89.87 (11) | O2—C6—C7' | 112.8 (4) |
| O1W$^{i}$—Ni1—O2W$^{i}$ | 91.93 (11) | O1—C6—C7 | 114.3 (4) |
| O1W—Ni1—O2W | 91.93 (11) | O2—C6—C7 | 119.7 (4) |
| O1W$^{i}$—Ni1—O2W | 89.87 (11) | C8—C7—C9 | 103.8 (8) |
| O2W$^{i}$—Ni1—O2W | 177.41 (16) | C8—C7—C6 | 106.4 (5) |
| O1W—Ni1—N1 | 173.17 (13) | C9—C7—C6 | 111.5 (5) |
| O1W$^{i}$—Ni1—N1 | 94.61 (13) | C8—C7—H7 | 111.6 |
| O2W$^{i}$—Ni1—N1 | 89.99 (11) | C9—C7—H7 | 111.6 |
| O2W—Ni1—N1 | 88.01 (11) | C6—C7—H7 | 111.6 |
| O1W—Ni1—N1$^{i}$ | 94.61 (13) | C7—C8—C9$^{ii}$ | 115.6 (6) |
| O1W$^{i}$—Ni1—N1$^{i}$ | 173.17 (13) | C7—C8—H8A | 108.4 |
| O2W$^{i}$—Ni1—N1$^{i}$ | 88.01 (11) | C9$^{ii}$—C8—H8A | 108.4 |
| O2W—Ni1—N1$^{i}$ | 89.98 (11) | C7—C8—H8B | 108.4 |
| N1—Ni1—N1$^{i}$ | 78.57 (18) | C9$^{ii}$—C8—H8B | 108.4 |
| Ni1—O1W—H1W | 124.2 | H8A—C8—H8B | 107.5 |
| Ni1—O1W—H2W | 121.8 | C8$^{ii}$—C9—C7 | 113.9 (6) |
| H1W—O1W—H2W | 110.8 | C8$^{ii}$—C9—H9A | 108.8 |
| Ni1—O2W—H3W | 127.6 | C7—C9—H9A | 108.8 |
| Ni1—O2W—H4W | 113.8 | C8$^{ii}$—C9—H9B | 108.8 |
| H3W—O2W—H4W | 113.4 | C7—C9—H9B | 108.8 |
| C5—N1—C1 | 118.8 (4) | H9A—C9—H9B | 107.7 |
| C5—N1—Ni1 | 126.2 (3) | C8'—C7'—C6 | 111.3 (5) |
| C1—N1—Ni1 | 115.0 (3) | C8'—C7'—C9' | 100.5 (8) |
| N1—C1—C2 | 120.8 (5) | C6—C7'—C9' | 105.1 (5) |
| N1—C1—C1$^{i}$ | 115.6 (2) | C8'—C7'—H7' | 113.0 |
| C2—C1—C1$^{i}$ | 123.6 (3) | C6—C7'—H7' | 113.0 |
| C3—C2—C1 | 120.2 (5) | C9'—C7'—H7' | 113.0 |
| C3—C2—H2 | 119.9 | C7'—C8'—C9'$^{ii}$ | 112.9 (6) |
| C1—C2—H2 | 119.9 | C7'—C8'—H8'1 | 109.0 |
| C4—C3—C2 | 119.0 (5) | C9'$^{ii}$—C8'—H8'1 | 109.0 |
| C4—C3—H3 | 120.5 | C7'—C8'—H8'2 | 109.0 |
| C2—C3—H3 | 120.5 | C9'$^{ii}$—C8'—H8'2 | 109.0 |
| C3—C4—C5 | 119.7 (5) | H8'1—C8'—H8'2 | 107.8 |
| C3—C4—H4 | 120.1 | C8'$^{ii}$—C9'—C7' | 117.5 (7) |

| | | | |
|---|---|---|---|
| C5—C4—H4 | 120.1 | C8$^{ii}$—C9'—H9'1 | 107.9 |
| N1—C5—C4 | 121.5 (5) | C7'—C9'—H9'1 | 107.9 |
| N1—C5—H5 | 119.3 | C8$^{ii}$—C9'—H9'2 | 107.9 |
| C4—C5—H5 | 119.3 | C7'—C9'—H9'2 | 107.9 |
| O1—C6—O2 | 123.7 (3) | H9'1—C9'—H9'2 | 107.2 |
| O1W$^{i}$—Ni1—N1—C5 | 0.8 (3) | O2—C6—C7—C8 | −128.8 (7) |
| O2W$^{i}$—Ni1—N1—C5 | −91.1 (3) | C7'—C6—C7—C8 | −49.2 (11) |
| O2W—Ni1—N1—C5 | 90.5 (3) | O1—C6—C7—C9 | −179.6 (8) |
| N1$^{i}$—Ni1—N1—C5 | −179.1 (4) | O2—C6—C7—C9 | −16.3 (11) |
| O1W$^{i}$—Ni1—N1—C1 | 178.9 (3) | C7'—C6—C7—C9 | 63.3 (12) |
| O2W$^{i}$—Ni1—N1—C1 | 86.9 (3) | C9—C7—C8—C9$^{ii}$ | 48.8 (10) |
| O2W—Ni1—N1—C1 | −91.4 (3) | C6—C7—C8—C9$^{ii}$ | 166.6 (9) |
| N1$^{i}$—Ni1—N1—C1 | −1.1 (2) | C8—C7—C9—C8$^{ii}$ | −58.2 (10) |
| C5—N1—C1—C2 | 1.5 (6) | C6—C7—C9—C8$^{ii}$ | −172.3 (9) |
| Ni1—N1—C1—C2 | −176.7 (4) | O1—C6—C7'—C8' | −11.3 (11) |
| C5—N1—C1—C1$^{i}$ | −179.0 (4) | O2—C6—C7'—C8' | 176.3 (7) |
| Ni1—N1—C1—C1$^{i}$ | 2.8 (5) | C7—C6—C7'—C8' | 64.2 (13) |
| N1—C1—C2—C3 | −0.6 (8) | O1—C6—C7'—C9' | −119.2 (8) |
| C1$^{i}$—C1—C2—C3 | 179.9 (5) | O2—C6—C7'—C9' | 68.4 (8) |
| C1—C2—C3—C4 | −0.2 (10) | C7—C6—C7'—C9' | −43.7 (10) |
| C2—C3—C4—C5 | 0.1 (10) | C6—C7'—C8'—C9'$^{ii}$ | −163.0 (9) |
| C1—N1—C5—C4 | −1.6 (6) | C9'—C7'—C8'—C9'$^{ii}$ | −52.0 (10) |
| Ni1—N1—C5—C4 | 176.3 (4) | C8'—C7'—C9'—C8'$^{ii}$ | 58.9 (10) |
| C3—C4—C5—N1 | 0.9 (8) | C6—C7'—C9'—C8'$^{ii}$ | 174.6 (10) |
| O1—C6—C7—C8 | 67.9 (9) | | |

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

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1W—H1W···O2$^{iii}$ | 0.81 | 2.00 | 2.759 (4) | 157 |
| O1W—H2W···O2$^{iv}$ | 0.81 | 1.83 | 2.637 (4) | 175 |
| O2W—H3W···O1 | 0.92 | 1.87 | 2.754 (4) | 162 |
| O2W—H4W···O1$^{v}$ | 0.89 | 1.79 | 2.678 (4) | 173 |

Symmetry codes: (iii) −*x*+1/2, −*y*+1/2, −*z*+1; (iv) *x*, *y*, *z*−1; (v) −*x*+1, *y*, −*z*+3/2.

**Fig. 1**

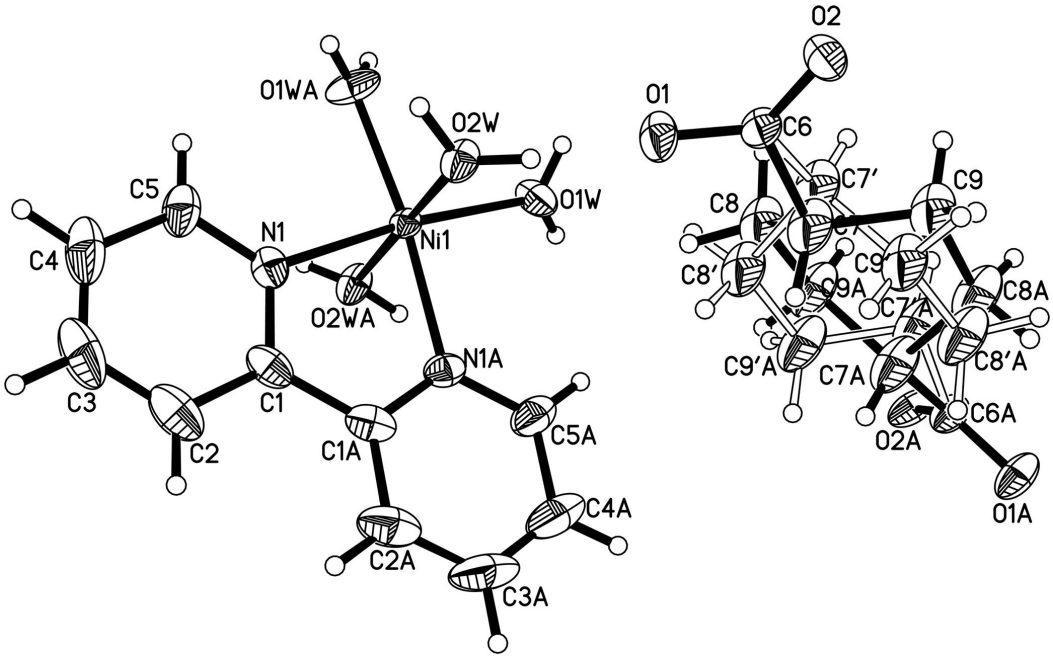
O1WA
O2W
O1W
C5
N1
Ni1
C4
O2WA
N1A
C3
C1
C5A
C2
C1A
C4A
C2A
C3A
O2
O1
C6
C7′
C9
C8
C8′
C9′
C9A
C8A
C7′A
C9′A
C7A
C8′A
C6A
O2A
O1A

**Fig. 2**

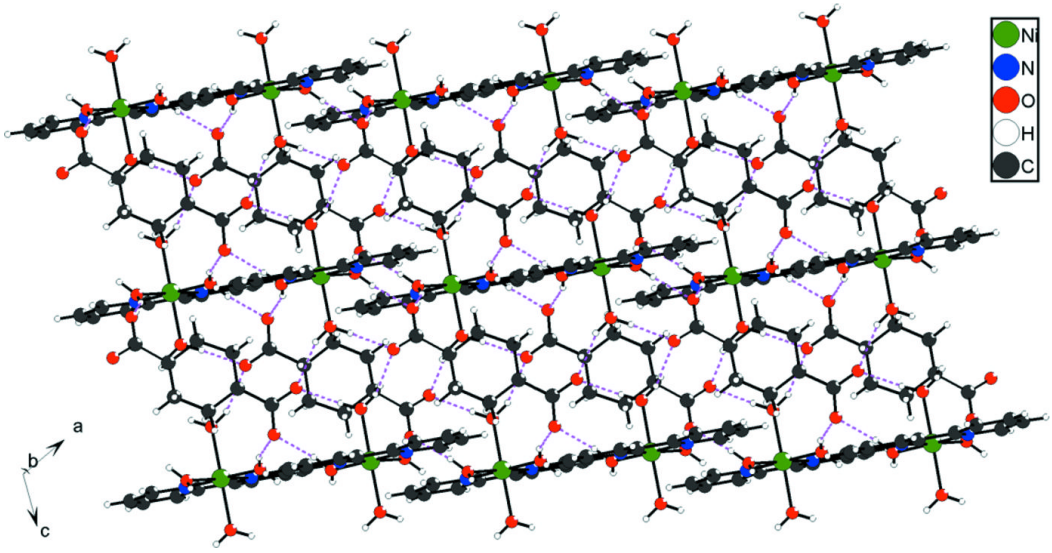

**Fig. 3**