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catena-Poly[[[(di-2-pyridylamine-$\kappa^2N^2,N^{2'}$)nickel(II)]-μ-carbonato-$\kappa^3O,O':O''$] trihydrate]

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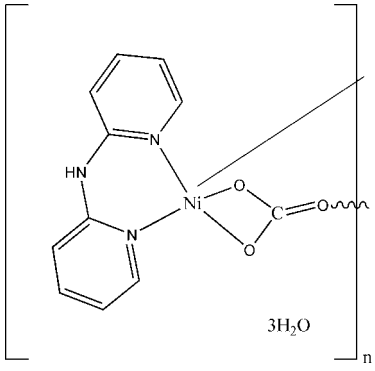
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.026; wR factor = 0.063; data-to-parameter ratio = 14.1.

In the title polymer, $\{[Ni(CO_3)(C_{10}H_9N_3)]\cdot 3H_2O\}_n$, each Ni^{II} atom is coordinated by three O atoms from two carbonate ligands and two N atoms from one bis(2-pyridyl)amine ligand, and has a distorted square-pyramidal geometry. The compound forms infinite chains *via* carbonate ligands bridging the [bis(2-pyridyl)amine]nickel(II) units which are further linked into neutral layers through N—H···O(carbonate) intermolecular hydrogen-bonding interactions. The water molecules form an infinite lamellar structure with an $R_5^5(10)$ graph-set motif. They occupy the space between the chains and are connected through O—H···O hydrogen bonds to the carbonate ligands. Furthermore, weak offset π–π stackings stabilize the packing network [the centroid-to-centroid distance is 3.674 (1) Å and the interplanar distance 3.438 Å].

Related literature

For related literature, see: Bernstein *et al.* (1995); Etter *et al.* (1990); Gu *et al.* (2004); Iglesias *et al.* (2003); Kim *et al.* (2003); Moulton & Zaworotko (2001).



Experimental

Crystal data

$[Ni(CO_3)(C_{10}H_9N_3)]\cdot 3H_2O$
M_r = 343.97
Monoclinic, $P2_1/c$
a = 11.2453 (11) Å
b = 7.1554 (7) Å
c = 17.3387 (16) Å
β = 101.106 (1)°
V = 1369.0 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.45 mm^{-1}
T = 298 (2) K
0.20 × 0.19 × 0.18 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan *SADABS* (Sheldrick, 1996)
T_{min} = 0.760, T_{max} = 0.780
7073 measured reflections
2671 independent reflections
2068 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.063
S = 0.99
2671 reflections
190 parameters
9 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O3^{i}	0.86	1.96	2.788 (2)	161
O4—H4A···O5	0.83	2.00	2.823 (3)	171
O4—H4B···O2^{ii}	0.84	1.98	2.797 (2)	165
O5—H5A···O6	0.82	1.97	2.754 (3)	158
O5—H5B···O1	0.84	1.95	2.790 (2)	171
O6—H6A···O5^{iii}	0.83	2.12	2.934 (2)	164
O6—H6B···O4^{iv}	0.84	1.91	2.735 (3)	171

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2174).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2004). *APEX2* (Version 1.27) and *SMART* (Version 7.23A). Bruker AXS Inc, Madison, Wisconsin, USA.
Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* B**46**, 256–262.
Gu, C.-S., Liu, J.-W., Huo, L.-H., Zhao, H., Zhao, J.-G. & Gao, S. (2004). *Acta Cryst.* E**60**, o760–o761.
Iglesias, S., Castillo, O., Luque, A. & Romaan, P. (2003). *Inorg. Chim. Acta*, **349**, 273–278.
Kim, J. C., Jo, H., Lough, A. J., Cho, J., Lee, U. & Pyun, S. Y. (2003). *Inorg. Chem. Commun.* **6**, 474–477.
Moulton, B. & Zaworotko, M. J. (2001). *Chem. Rev.* **101**, 1629–1658.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany

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supplementary materials

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catena-Poly[[[(di-2-pyridylamine-$\kappa^2N^2,N^{2'}$)nickel(II)]-μ-carbonato-$\kappa^3O,O':O''$] trihydrate]

X.-L. You and L.-H. Wang

Comment

Molecular self-assembly of supramolecular architectures has received much attention during recent decades (Kim *et al.*, 2003; Iglesias *et al.*, 2003; Moulton & Zaworotko, 2001). The structures and properties of such systems depend on the coordination and geometric preferences of both the central metals ions and bridging building blocks as well as the influence of weaker non-covalent interactions, such as hydrogen bonds and π-π stacking interactions. 4-Chlorobenzoic acid and imidazole are excellent candidates for the construction of supramolecular complexes, since they not only have multiple coordination modes but also can form regular hydrogen bonds by functioning as both hydrogen-bond donor and acceptor (Gu *et al.*, 2004). Recently, we obtained the title polymer nickel complex (I) by the reaction of nickel carbonate, bis(2-pyridyl)amine in solution of methanol and acetonitrile.

In complex (I), each Ni^{II} centre is coordinated by three O atoms from two carbonate ligands, two N atoms from one bis(2-pyridyl)amine ligand, and displayed a distorted square pyramidal geometry (Fig. 1). The compound forms infinite chain *via* carbonate ligands bridging the Ni-bis(2-pyridyl)amine units and further linked into a neutral layer through N3—H···O3(carbonate) intermolecular hydrogen bonding interactions (Table 1) and weak slipped π-π stacking with centroid to centroid distance of 3.674 (1)Å and interplanar distance of 3.438\%A between pyridyl group of neighboring chain. The water molecules form infinite lamellar structure containing $R^5_5(10)$ graph set motif (Etter *et al.*, 1990; Bernstein *et al.*, 1995), which fill in the space between the chains and are connected through O—H···O hydrogen bonds with carbonate ligands (Table 1).

Experimental

bis(2-pyridyl)amine(0.065 g, 7 mmol), $Ni(CH3COO)_2$ (0.18 g, 12 mmol) and Na_2CO_3(0.23 g,10 mmol), were added in a mixed solvent of methanol and acetonitrile, the mixture was heated for five h under reflux. during the process stirring and influx were required. The resultant was then filtered to give a pure solution which was infiltrated by diethyl ether freely in a closed vessel, a weeks later some single crystals of the size suitable for X-Ray diffraction analysis.

Refinement

H atoms attached to C and N atoms were placed at calculated positions and treated as riding on their parent atoms with C—H = 0.93 Å, N—H = 0.86 Å and with U_{iso}(H) = 1.2 U_{eq}(C, N). H atoms attached to water molecules were located in difference Fourier maps but were treated as riding with O—H distance restraints to 0.82 Å and H···H to 1.39 Å and with U_{iso}(H)= 1.5 U_{eq}(O).

Figures

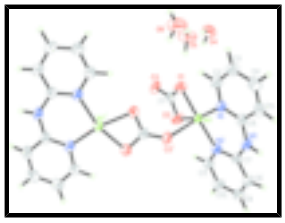


Fig. 1. The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii. [Symmetry code: (i) 2 − *x*, 1/2 + *y*, 1/2 − *z*].

catena-Poly[[[(di-2-pyridylamine-κ^2*N*^{2},*N*$^{2'}$)nickel(II)]- μ-carbonato-κ^3*O*,*O*':*O*''] trihydrate]

Crystal data

$[Ni(CO_3)(C_{10}H_9N_3)]\cdot 3H_2O$	F_{000} = 712
M_r = 343.97	D_x = 1.669 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2600 reflections
a = 11.2453 (11) Å	θ = 1.7–26.0º
b = 7.1554 (7) Å	μ = 1.45 mm^{-1}
c = 17.3387 (16) Å	*T* = 298 (2) K
β = 101.1060 (10)º	Block, blue
V = 1369.0 (2) Å^3	0.20 × 0.19 × 0.18 mm
Z = 4	

Data collection

Bruker APEX-II area-detector diffractometer	2671 independent reflections
Radiation source: fine-focus sealed tube	2068 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 298(2) K	θ_{max} = 26.0º
φ and ω scan	θ_{min} = 1.9º
Absorption correction: multi-scan SADABS (Sheldrick, 1996)	*h* = −13→13
T_{min} = 0.760, T_{max} = 0.780	*k* = −8→8
7073 measured reflections	*l* = −16→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.027	H-atom parameters constrained
$wR(F^2)$ = 0.063	$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.99	$(\Delta/\sigma)_{max}$ = 0.001

2671 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
190 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-3}
9 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.96874 (2)	0.68093 (3)	0.128525 (13)	0.02662 (9)
N2	1.08891 (15)	0.6870 (2)	0.05901 (9)	0.0305 (4)
N3	0.95476 (15)	0.8085 (2)	−0.05193 (9)	0.0359 (4)
H3	0.9528	0.8552	−0.0979	0.043*
O1	0.87293 (12)	0.5970 (2)	0.20646 (8)	0.0398 (4)
N1	0.83439 (15)	0.7605 (2)	0.04433 (9)	0.0311 (4)
C6	0.84388 (18)	0.8087 (3)	−0.02909 (11)	0.0311 (4)
O2	1.06489 (12)	0.5455 (2)	0.21974 (8)	0.0442 (4)
C7	1.06774 (18)	0.7483 (3)	−0.01579 (11)	0.0308 (5)
C3	0.6207 (2)	0.8162 (3)	0.01007 (13)	0.0456 (6)
H3A	0.5456	0.8181	0.0250	0.055*
C11	1.20373 (19)	0.6317 (3)	0.09050 (13)	0.0388 (5)
H11	1.2195	0.5891	0.1421	0.047*
C9	1.2734 (2)	0.6984 (3)	−0.02676 (13)	0.0429 (6)
H9	1.3351	0.7020	−0.0555	0.051*
C8	1.1593 (2)	0.7546 (3)	−0.05985 (12)	0.0386 (5)
H8	1.1425	0.7970	−0.1115	0.046*
C1	0.96998 (18)	0.5327 (3)	0.25138 (11)	0.0308 (5)
C2	0.72183 (19)	0.7660 (3)	0.06210 (12)	0.0372 (5)
H2	0.7137	0.7336	0.1128	0.045*
C10	1.2966 (2)	0.6354 (3)	0.05080 (13)	0.0415 (5)
H10	1.3739	0.5968	0.0748	0.050*
C5	0.7433 (2)	0.8611 (3)	−0.08549 (13)	0.0430 (6)
H5	0.7525	0.8932	−0.1360	0.052*
O3	0.97143 (13)	0.46848 (19)	0.31877 (8)	0.0387 (4)
O4	0.69188 (15)	0.0454 (3)	0.20442 (10)	0.0679 (5)
H4A	0.6744	0.1583	0.2043	0.102*

H4B	0.7660	0.0306	0.2211	0.102*
O5	0.65269 (16)	0.4323 (3)	0.21925 (11)	0.0731 (6)
H5A	0.6025	0.5150	0.2043	0.110*
H5B	0.7226	0.4699	0.2157	0.110*
O6	0.52597 (17)	0.7637 (3)	0.19881 (12)	0.0799 (6)
H6A	0.4651	0.8016	0.2150	0.120*
H6B	0.5797	0.8459	0.2053	0.120*
C4	0.6314 (2)	0.8648 (3)	−0.06583 (14)	0.0474 (6)
H4	0.5635	0.8993	−0.1027	0.057*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.02843 (15)	0.03306 (16)	0.01923 (14)	0.00066 (11)	0.00676 (10)	0.00453 (11)
N2	0.0360 (9)	0.0311 (9)	0.0249 (9)	−0.0002 (8)	0.0069 (7)	0.0007 (7)
N3	0.0410 (10)	0.0451 (11)	0.0222 (9)	0.0009 (8)	0.0072 (7)	0.0074 (8)
O1	0.0331 (8)	0.0548 (10)	0.0316 (8)	0.0015 (7)	0.0065 (6)	0.0109 (7)
N1	0.0355 (9)	0.0323 (9)	0.0266 (9)	−0.0017 (7)	0.0086 (7)	0.0003 (7)
C6	0.0394 (11)	0.0285 (11)	0.0255 (10)	−0.0011 (9)	0.0066 (8)	−0.0001 (9)
O2	0.0377 (8)	0.0619 (11)	0.0355 (8)	0.0077 (7)	0.0131 (7)	0.0173 (7)
C7	0.0392 (12)	0.0257 (10)	0.0286 (11)	−0.0026 (9)	0.0097 (9)	−0.0024 (9)
C3	0.0377 (13)	0.0528 (15)	0.0466 (14)	0.0057 (11)	0.0086 (10)	0.0048 (12)
C11	0.0411 (12)	0.0445 (14)	0.0309 (12)	0.0016 (10)	0.0070 (10)	0.0003 (10)
C9	0.0413 (13)	0.0483 (15)	0.0437 (13)	−0.0053 (11)	0.0198 (10)	−0.0038 (11)
C8	0.0476 (13)	0.0413 (12)	0.0303 (12)	−0.0040 (10)	0.0159 (10)	0.0011 (10)
C1	0.0418 (12)	0.0275 (11)	0.0242 (11)	−0.0014 (9)	0.0089 (9)	−0.0019 (9)
C2	0.0382 (12)	0.0420 (13)	0.0333 (12)	0.0018 (10)	0.0117 (10)	0.0052 (10)
C10	0.0362 (12)	0.0477 (14)	0.0416 (13)	0.0010 (10)	0.0102 (10)	−0.0011 (11)
C5	0.0527 (14)	0.0453 (14)	0.0291 (12)	0.0024 (11)	0.0031 (10)	0.0078 (10)
O3	0.0559 (9)	0.0366 (8)	0.0253 (8)	0.0049 (7)	0.0118 (7)	0.0044 (6)
O4	0.0499 (10)	0.0764 (14)	0.0763 (13)	−0.0059 (9)	0.0096 (9)	−0.0186 (10)
O5	0.0521 (11)	0.0642 (13)	0.1086 (17)	−0.0082 (9)	0.0295 (11)	0.0081 (11)
O6	0.0583 (12)	0.0697 (13)	0.1189 (18)	−0.0003 (10)	0.0345 (12)	−0.0102 (12)
C4	0.0397 (13)	0.0547 (16)	0.0446 (14)	0.0085 (11)	0.0002 (11)	0.0083 (11)

Geometric parameters (Å, °)

Ni1—N1	1.9718 (17)	C11—C10	1.357 (3)
Ni1—O1	1.9769 (13)	C11—H11	0.9300
Ni1—N2	1.9770 (16)	C9—C8	1.361 (3)
Ni1—O2	1.9877 (14)	C9—C10	1.395 (3)
Ni1—O3^{i}	2.2988 (14)	C9—H9	0.9300
Ni1—C1	2.3772 (19)	C8—H8	0.9300
N2—C7	1.346 (2)	C1—O3	1.253 (2)
N2—C11	1.360 (3)	C2—H2	0.9300
N3—C7	1.373 (2)	C10—H10	0.9300
N3—C6	1.379 (2)	C5—C4	1.366 (3)
N3—H3	0.8600	C5—H5	0.9300

O1—C1	1.297 (2)	O3—Ni1^{ii}	2.2988 (14)
N1—C6	1.343 (2)	O4—H4A	0.8316
N1—C2	1.360 (2)	O4—H4B	0.8353
C6—C5	1.396 (3)	O5—H5A	0.8244
O2—C1	1.294 (2)	O5—H5B	0.8446
C7—C8	1.396 (3)	O6—H6A	0.8328
C3—C2	1.357 (3)	O6—H6B	0.8352
C3—C4	1.389 (3)	C4—H4	0.9300
C3—H3A	0.9300		
N1—Ni1—O1	98.81 (6)	C2—C3—H3A	120.6
N1—Ni1—N2	93.36 (7)	C4—C3—H3A	120.6
O1—Ni1—N2	161.80 (6)	C10—C11—N2	123.7 (2)
N1—Ni1—O2	162.12 (6)	C10—C11—H11	118.2
O1—Ni1—O2	65.96 (6)	N2—C11—H11	118.2
N2—Ni1—O2	99.49 (6)	C8—C9—C10	119.2 (2)
N1—Ni1—O3^{i}	99.19 (6)	C8—C9—H9	120.4
O1—Ni1—O3^{i}	99.00 (6)	C10—C9—H9	120.4
N2—Ni1—O3^{i}	92.33 (6)	C9—C8—C7	119.6 (2)
O2—Ni1—O3^{i}	92.71 (6)	C9—C8—H8	120.2
N1—Ni1—C1	131.58 (7)	C7—C8—H8	120.2
O1—Ni1—C1	33.06 (6)	O3—C1—O2	123.91 (19)
N2—Ni1—C1	132.02 (7)	O3—C1—O1	123.26 (18)
O2—Ni1—C1	32.97 (6)	O2—C1—O1	112.82 (17)
O3^{i}—Ni1—C1	95.30 (6)	O3—C1—Ni1	175.00 (15)
C7—N2—C11	117.36 (17)	O2—C1—Ni1	56.73 (10)
C7—N2—Ni1	125.43 (14)	O1—C1—Ni1	56.26 (9)
C11—N2—Ni1	117.16 (13)	C3—C2—N1	123.67 (19)
C7—N3—C6	132.66 (17)	C3—C2—H2	118.2
C7—N3—H3	113.7	N1—C2—H2	118.2
C6—N3—H3	113.7	C11—C10—C9	118.4 (2)
C1—O1—Ni1	90.68 (11)	C11—C10—H10	120.8
C6—N1—C2	117.05 (17)	C9—C10—H10	120.8
C6—N1—Ni1	125.91 (14)	C4—C5—C6	119.4 (2)
C2—N1—Ni1	117.03 (13)	C4—C5—H5	120.3
N1—C6—N3	120.88 (18)	C6—C5—H5	120.3
N1—C6—C5	122.10 (19)	C1—O3—Ni1^{ii}	130.49 (12)
N3—C6—C5	117.02 (18)	H4A—O4—H4B	110.1
C1—O2—Ni1	90.29 (12)	H5A—O5—H5B	109.8
N2—C7—N3	121.21 (17)	H6A—O6—H6B	110.2
N2—C7—C8	121.70 (19)	C5—C4—C3	118.9 (2)
N3—C7—C8	117.09 (18)	C5—C4—H4	120.5
C2—C3—C4	118.8 (2)	C3—C4—H4	120.5

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

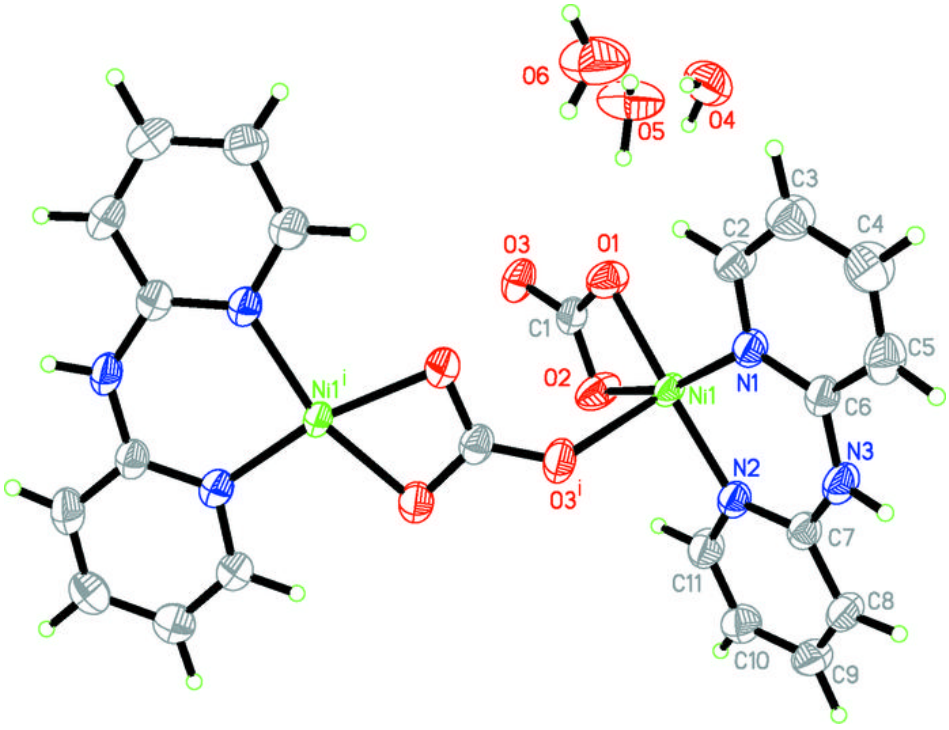
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N3—H3···O3^{iii}	0.86	1.96	2.788 (2)	161
O4—H4A···O5	0.83	2.00	2.823 (3)	171
O4—H4B···O2^{ii}	0.84	1.98	2.797 (2)	165
O5—H5A···O6	0.82	1.97	2.754 (3)	158
O5—H5B···O1	0.84	1.95	2.790 (2)	171
O6—H6A···O5^{iv}	0.83	2.12	2.934 (2)	164
O6—H6B···O4^{v}	0.84	1.91	2.735 (3)	171

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

Fig. 1


O6
O5
O4
C3
C2
C4
O3
O1
C1
C5
O2
Ni1
N1
C6
Ni1 i
N3
N2
O3 i
C7
C11
C8
C10
C9