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catena-Poly[[[[3-(2-pyridyl)-1*H*-pyrazole]nickel(II)]-μ-oxalato] sesquihydrate]

Bin Jiang[a] and Zhilu Liu[b]*

[a]Department of Pharmacy, Shandong Medical College, Jinan 250002, People's Republic of China, and [b]State Key Laboratory of Solid Lubrication, Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, Lanzhou 73000, People's Republic of China
Correspondence e-mail: liuzhilu2009@yahoo.com.cn

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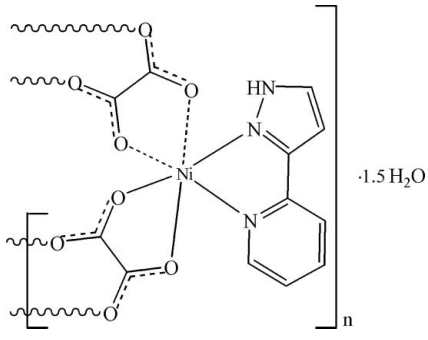
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.014 Å; R factor = 0.056; wR factor = 0.139; data-to-parameter ratio = 12.7.

In the title compound, $\{[Ni(C_2O_4)(C_8H_7N_3)]\cdot 1.5H_2O\}_n$, both unique Ni^{II} ions are chelated by an O,O'-bidentate oxalate ion and an N,N'-bidentate 3-(2-pyridyl)pyrazole molecule. A second, symmetry-generated, oxalate ion completes a distorted *cis*-NiN_2O_4 octahedral geometry for both metal centres. The bridging oxalate ions result in two distinct wave-like polymeric chains propagating in [100]. The packing is consolidated by N—H···O and O—H···O hydrogen bonds. The crystal studied was found to be an inversion twin.

Related literature

For related literature on coordination polymers, see: Ward (2007).



Experimental

Crystal data

$[Ni(C_2O_4)(C_8H_7N_3)]\cdot 1.5H_2O$
M_r = 318.92
Orthorhombic, $Pna2_1$
a = 9.763 (2) Å
b = 9.1970 (18) Å
c = 29.352 (6) Å
V = 2635.5 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.50 mm^{-1}
T = 293 K
0.12 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.841, T_{max} = 0.890
17815 measured reflections
4882 independent reflections
3723 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.139
S = 1.00
4882 reflections
385 parameters
12 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}
Absolute structure: Flack (1983), 2287 Friedel pairs
Flack parameter: 0.50 (3)

Table 1
Selected bond lengths (Å).

Ni1—O1	2.152 (5)	Ni2—O6	2.159 (6)
Ni1—O3	2.200 (6)	Ni2—O8	2.188 (4)
Ni1—O2^{i}	2.163 (6)	Ni2—O5^{ii}	2.142 (4)
Ni1—O4^{i}	2.177 (4)	Ni2—O7^{ii}	2.217 (6)
Ni1—N1	2.259 (6)	Ni2—N4	2.285 (6)
Ni1—N2	2.230 (6)	Ni2—N5	2.205 (6)

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{5}{2}, z$; (ii) $x+\frac{1}{2}, -y-\frac{1}{2}, z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O11^{iii}	0.97 (4)	1.81 (2)	2.745 (10)	160 (5)
N6—H6A···O10^{iv}	0.98 (16)	2.0 (2)	2.732 (9)	133 (5)
O9—H2W···O7^{v}	0.82 (4)	2.02 (4)	2.822 (9)	166 (6)
O9—H1W···O11^{vi}	0.82 (12)	2.22 (15)	2.813 (11)	130 (16)
O10—H3W···O4^{vii}	0.82 (5)	2.30 (7)	2.834 (9)	123 (7)
O10—H4W···O9^{vi}	0.82 (4)	2.08 (3)	2.811 (11)	148 (5)
O11—H5W···O9^{viii}	0.82 (5)	2.15 (4)	2.813 (11)	138 (5)
O11—H6W···O8^{ix}	0.82 (4)	2.17 (4)	2.876 (9)	144 (6)

Symmetry codes: (iii) $-x+1, -y+2, z+\frac{1}{2}$; (iv) $x, y-1, z$; (v) $x+\frac{1}{2}, -y+\frac{1}{2}, z$; (vi) $x+\frac{1}{2}, -y+\frac{3}{2}, z$; (vii) $-x+\frac{3}{2}, y-\frac{1}{2}, z-\frac{1}{2}$; (viii) $x-\frac{1}{2}, -y+\frac{3}{2}, z$; (ix) $x, y+1, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5014).

References

Bruker (2004). *APEX2*, *SAINT-Plus* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Ward, M. D. (2007). *Coord. Chem. Rev.* **251**, 1663–1677.

supplementary materials

Acta Cryst. (2009). E**65**, m898-m899 [**doi:10.1107/S1600536809026117**]

catena-Poly[[[[3-(2-pyridyl)-1*H*-pyrazole]nickel(II)]-μ-oxalato] sesquihydrate]

B. Jiang and Z. Liu

Comment

As part of our ongoing studies of coordination polymers (Ward, 2007), we now report the synthesis and crystal structural characterization of the title compound, (I).

The N^{II} ions are hexcoordianted, chelated by two oxalate and one 3-(2-pyridyl)pyrazole ligand (Table 1). While each oxalate ligand acts as one bridige to chalate two Ni ions, forming one wave-like line with Ni···Ni distance being 5.562 Å, shown in Figure 2. The structure is consolidated by N—H···O and O—H···O hydrogen bonds (Table 2, Figure 3).

Experimental

The synthesis was performed in a 25 ml Teflon-lined stainless steel vessel: $NiCl_2$ (1 mmol), 3-(2-pyridyl)pyrazole (1 mmol), oxalic acid (1 mmol), and H_2O (10 ml) were mixed and heated to 433 K for three days. On cooling, green blocks of (I) were recovered. Anal. Calc. for $C_{20}H_{20}Ni_2N_6O_{11}$: C 37.60, H 3.13, N 13.16%; Found: 37.56, H 3.06, N 13.10%.

Refinement

The C-bound H atoms were geometrically planced (C—H = 0.93Å) and refined as riding with $U_{iso} = 1.2U_{eq}$(C). The N- and O-bound H atoms were located in difference maps and refined with distance restraints: N—H = 0.97 (1)Å, O—H = 0.82 (2)Å, H···H = 1.38 (2)Å.

Figures

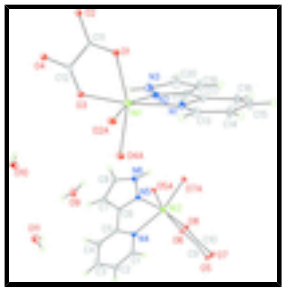


Fig. 1. A view of (I) with the unique atoms labelled. Displacement ellipsoids are drawn at the 30% probability level.

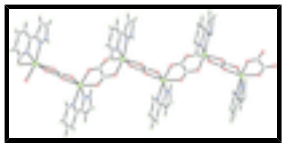


Fig. 2. A view of the chain strcuture of (I).

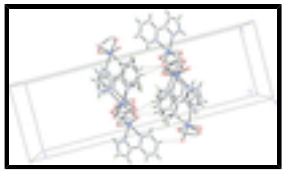


Fig. 3. A view of the packing strcuture of (I).

catena-Poly[[[[3-(2-pyridyl)-1<>H-pyrazole]nickel(II)]-μ-oxalato] sesquihydrate]

Crystal data

$[Ni(C_2O_4)(C_8H_7N_3)]\cdot 1.5H_2O$	F_{000} = 1304
M_r = 318.92	D_x = 1.607 Mg m^{-3}
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: P 2c -2n	Cell parameters from 4779 reflections
a = 9.763 (2) Å	θ = 2.3–25.5º
b = 9.1970 (18) Å	μ = 1.50 mm^{-1}
c = 29.352 (6) Å	T = 293 K
V = 2635.5 (9) Å^3	Block, green
Z = 8	0.12 × 0.10 × 0.08 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	4882 independent reflections
Radiation source: fine-focus sealed tube	3723 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.059
T = 293 K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Bruker, 2004)	h = −11→11
T_{min} = 0.841, T_{max} = 0.890	k = −11→10
17815 measured reflections	l = −35→35

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.056	$w = 1/[\sigma^2(F_o^2) + (0.078P)^2 + 0.5477P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.139	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.00	$\Delta\rho_{max}$ = 0.47 e Å^{-3}
4882 reflections	$\Delta\rho_{min}$ = −0.36 e Å^{-3}
385 parameters	Extinction correction: none
12 restraints	Absolute structure: Flack (1983), 2287 Friedel pairs

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Flack parameter: 0.50 (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	0.31148 (9)	1.09616 (9)	0.84957 (7)	0.0406 (2)
Ni2	0.55514 (8)	−0.09515 (9)	0.08796 (7)	0.0408 (2)
C1	0.3921 (9)	0.0950 (8)	0.0119 (3)	0.049 (2)
H1	0.3731	0.0049	−0.0010	0.059*
C2	0.3379 (10)	0.2187 (11)	−0.0082 (4)	0.062 (2)
H2	0.2809	0.2111	−0.0335	0.074*
C3	0.3688 (12)	0.3506 (12)	0.0094 (3)	0.077 (4)
H3	0.3325	0.4349	−0.0033	0.092*
C4	0.4564 (11)	0.3578 (10)	0.0472 (4)	0.060 (3)
H4	0.4850	0.4472	0.0585	0.073*
C5	0.4996 (10)	0.2304 (8)	0.0671 (3)	0.041 (2)
C6	0.5898 (9)	0.2314 (8)	0.1082 (3)	0.036 (2)
C7	0.6452 (10)	0.3438 (9)	0.1323 (4)	0.062 (3)
H7	0.6355	0.4430	0.1270	0.075*
C8	0.7179 (10)	0.2767 (11)	0.1658 (4)	0.061 (3)
H8	0.7664	0.3233	0.1888	0.073*
C9	0.3240 (8)	−0.2826 (8)	0.0649 (3)	0.0342 (19)
C10	0.2918 (7)	−0.2229 (7)	0.1133 (3)	0.0254 (15)
C11	0.5767 (6)	1.2152 (8)	0.8712 (2)	0.0236 (13)
C12	0.5476 (8)	1.2747 (8)	0.8228 (3)	0.0325 (18)
C13	0.1336 (9)	0.9194 (11)	0.9256 (3)	0.057 (2)
H13	0.1073	1.0111	0.9357	0.069*
C14	0.0855 (11)	0.7996 (12)	0.9485 (3)	0.071 (3)
H14	0.0292	0.8096	0.9738	0.085*
C15	0.1225 (10)	0.6663 (12)	0.9331 (4)	0.070 (3)
H15	0.0937	0.5844	0.9490	0.084*
C16	0.1990 (10)	0.6493 (10)	0.8960 (4)	0.060 (3)
H16	0.2158	0.5570	0.8843	0.072*
C17	0.2534 (9)	0.7723 (8)	0.8749 (3)	0.0372 (19)
C18	0.3377 (9)	0.7695 (8)	0.8356 (3)	0.040 (2)

C19	0.3938 (12)	0.6511 (11)	0.8106 (4)	0.071 (3)
H19	0.3789	0.5526	0.8157	0.085*
C20	0.4713 (14)	0.7090 (12)	0.7784 (5)	0.088 (4)
H20	0.5256	0.6582	0.7579	0.106*
N1	0.2170 (6)	0.9107 (6)	0.8890 (2)	0.0378 (15)
N2	0.3773 (6)	0.8926 (7)	0.8146 (2)	0.0384 (15)
N3	0.4576 (7)	0.8577 (8)	0.7808 (2)	0.0516 (18)
N4	0.4710 (6)	0.1009 (6)	0.0492 (2)	0.0353 (14)
N5	0.6263 (6)	0.1013 (7)	0.1239 (2)	0.0375 (14)
N6	0.7085 (8)	0.1366 (9)	0.1604 (2)	0.0536 (19)
O1	0.4923 (5)	1.1355 (5)	0.88962 (16)	0.0351 (10)
O2	0.6957 (5)	1.2463 (5)	0.8884 (3)	0.0398 (17)
O3	0.4389 (5)	1.2387 (5)	0.8069 (2)	0.0347 (16)
O4	0.6367 (5)	1.3553 (5)	0.80613 (16)	0.0354 (10)
O5	0.2318 (4)	−0.3592 (5)	0.04713 (16)	0.0335 (10)
O6	0.4326 (5)	−0.2429 (5)	0.0479 (3)	0.0378 (17)
O7	0.1787 (6)	−0.2608 (6)	0.1324 (2)	0.0385 (17)
O8	0.3784 (4)	−0.1410 (5)	0.13145 (17)	0.0383 (11)
O9	0.6278 (8)	0.6448 (6)	0.2198 (2)	0.0605 (12)
O10	0.8552 (8)	0.9517 (8)	0.2145 (2)	0.0727 (17)
O11	0.3970 (8)	0.9636 (7)	0.2236 (2)	0.0667 (16)
H6W	0.412 (4)	0.905 (5)	0.2033 (15)	0.077 (17)*
H2W	0.632 (6)	0.689 (6)	0.1956 (11)	0.074 (19)*
H1W	0.672 (16)	0.569 (10)	0.221 (3)	0.083 (10)*
H3W	0.860 (5)	0.989 (8)	0.2399 (12)	0.085 (2)*
H4W	0.927 (3)	0.918 (7)	0.2051 (17)	0.093 (2)*
H5W	0.321 (4)	0.957 (7)	0.235 (3)	0.107 (4)*
H3A	0.490 (5)	0.935 (4)	0.7611 (14)	0.064 (13)*
H6A	0.71 (3)	0.069 (18)	0.186 (5)	0.059 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0366 (4)	0.0418 (5)	0.0432 (5)	−0.0004 (4)	0.0012 (4)	0.0039 (5)
Ni2	0.0352 (4)	0.0420 (5)	0.0453 (5)	0.0012 (4)	−0.0004 (4)	−0.0020 (5)
C1	0.064 (5)	0.039 (4)	0.045 (4)	0.017 (4)	−0.007 (4)	−0.010 (3)
C2	0.070 (6)	0.072 (6)	0.044 (5)	0.024 (5)	−0.019 (4)	−0.002 (5)
C3	0.116 (9)	0.074 (7)	0.041 (5)	0.056 (6)	−0.014 (5)	0.004 (5)
C4	0.092 (7)	0.037 (5)	0.053 (5)	0.014 (4)	−0.001 (5)	−0.008 (4)
C5	0.047 (5)	0.039 (4)	0.039 (5)	0.016 (4)	0.012 (4)	0.007 (3)
C6	0.043 (4)	0.030 (4)	0.035 (5)	0.005 (3)	−0.016 (3)	0.005 (3)
C7	0.081 (6)	0.024 (4)	0.082 (7)	−0.015 (4)	−0.021 (6)	−0.010 (4)
C8	0.062 (5)	0.057 (5)	0.062 (6)	−0.012 (5)	−0.037 (5)	−0.015 (5)
C9	0.051 (5)	0.024 (3)	0.028 (4)	0.025 (4)	0.000 (3)	−0.011 (3)
C10	0.016 (3)	0.031 (3)	0.029 (4)	−0.002 (3)	0.002 (3)	0.000 (3)
C11	0.016 (3)	0.027 (3)	0.028 (3)	−0.016 (3)	−0.002 (2)	−0.002 (3)
C12	0.037 (5)	0.031 (3)	0.029 (4)	0.010 (3)	0.005 (3)	0.007 (3)
C13	0.060 (5)	0.077 (6)	0.035 (4)	−0.011 (4)	0.008 (4)	−0.001 (4)

C14	0.095 (7)	0.082 (7)	0.035 (5)	−0.046 (7)	0.021 (5)	0.007 (5)
C15	0.082 (7)	0.055 (6)	0.071 (7)	−0.026 (5)	0.006 (5)	0.033 (5)
C16	0.065 (5)	0.033 (5)	0.083 (7)	−0.018 (4)	0.010 (5)	0.017 (5)
C17	0.044 (5)	0.031 (4)	0.038 (5)	−0.005 (3)	0.005 (4)	0.001 (3)
C18	0.036 (4)	0.031 (4)	0.051 (6)	0.000 (3)	−0.011 (4)	−0.004 (3)
C19	0.096 (8)	0.038 (5)	0.079 (7)	−0.002 (5)	0.024 (6)	0.006 (5)
C20	0.124 (10)	0.046 (5)	0.095 (10)	0.030 (7)	0.036 (8)	−0.023 (7)
N1	0.043 (3)	0.035 (4)	0.036 (3)	−0.002 (2)	0.006 (3)	0.004 (3)
N2	0.037 (3)	0.034 (3)	0.044 (3)	0.006 (2)	0.005 (3)	0.003 (3)
N3	0.050 (4)	0.047 (4)	0.058 (5)	0.009 (3)	0.019 (3)	−0.001 (3)
N4	0.035 (3)	0.037 (3)	0.034 (3)	0.016 (2)	−0.006 (2)	−0.007 (3)
N5	0.041 (3)	0.036 (3)	0.036 (3)	0.000 (3)	−0.014 (3)	−0.004 (3)
N6	0.061 (4)	0.058 (5)	0.042 (4)	−0.005 (3)	−0.027 (3)	0.000 (3)
O1	0.034 (2)	0.043 (3)	0.029 (2)	−0.001 (2)	−0.004 (2)	0.009 (2)
O2	0.042 (4)	0.042 (4)	0.035 (4)	−0.009 (2)	−0.019 (3)	0.0142 (19)
O3	0.023 (3)	0.045 (4)	0.036 (4)	−0.0085 (19)	−0.005 (2)	0.012 (2)
O4	0.034 (2)	0.041 (3)	0.031 (2)	−0.009 (2)	−0.0058 (19)	0.008 (2)
O5	0.030 (2)	0.039 (2)	0.032 (2)	−0.006 (2)	0.006 (2)	−0.011 (2)
O6	0.022 (3)	0.056 (4)	0.036 (4)	−0.0070 (19)	0.006 (2)	−0.018 (2)
O7	0.035 (3)	0.054 (4)	0.026 (4)	−0.015 (2)	0.016 (2)	−0.008 (2)
O8	0.028 (2)	0.052 (3)	0.035 (3)	−0.005 (2)	0.003 (2)	−0.016 (2)
O9	0.090 (4)	0.057 (3)	0.034 (2)	−0.003 (4)	0.015 (2)	0.007 (3)
O10	0.078 (5)	0.096 (5)	0.043 (4)	0.011 (4)	−0.014 (4)	0.017 (4)
O11	0.084 (5)	0.071 (4)	0.045 (4)	−0.006 (4)	−0.011 (4)	−0.005 (3)

Geometric parameters (Å, °)

Ni1—O1	2.152 (5)	C11—O2	1.299 (8)
Ni1—O3	2.200 (6)	C11—C12	1.550 (11)
Ni1—O2^{i}	2.163 (6)	C12—O3	1.206 (10)
Ni1—O4^{i}	2.177 (4)	C12—O4	1.243 (9)
Ni1—N1	2.259 (6)	C13—N1	1.349 (11)
Ni1—N2	2.230 (6)	C13—C14	1.374 (12)
Ni2—O6	2.159 (6)	C13—H13	0.9300
Ni2—O8	2.188 (4)	C14—C15	1.355 (16)
Ni2—O5^{ii}	2.142 (4)	C14—H14	0.9300
Ni2—O7^{ii}	2.217 (6)	C15—C16	1.330 (15)
Ni2—N4	2.285 (6)	C15—H15	0.9300
Ni2—N5	2.205 (6)	C16—C17	1.395 (11)
C1—N4	1.340 (11)	C16—H16	0.9300
C1—C2	1.386 (11)	C17—N1	1.385 (10)
C1—H1	0.9300	C17—C18	1.416 (13)
C2—C3	1.353 (14)	C18—N2	1.346 (10)
C2—H2	0.9300	C18—C19	1.424 (13)
C3—C4	1.401 (15)	C19—C20	1.321 (17)
C3—H3	0.9300	C19—H19	0.9300
C4—C5	1.376 (12)	C20—N3	1.376 (12)
C4—H4	0.9300	C20—H20	0.9300

C5—N4	1.331 (10)	N2—N3	1.304 (9)
C5—C6	1.494 (13)	N3—H3A	0.97 (4)
C6—N5	1.331 (9)	N5—N6	1.376 (9)
C6—C7	1.363 (12)	N6—H6A	0.98 (16)
C7—C8	1.362 (15)	O2—Ni1^{iii}	2.163 (6)
C7—H7	0.9300	O4—Ni1^{iii}	2.177 (4)
C8—N6	1.301 (11)	O5—Ni2^{iv}	2.142 (4)
C8—H8	0.9300	O7—Ni2^{iv}	2.217 (6)
C9—O6	1.227 (9)	O9—H2W	0.82 (4)
C9—O5	1.257 (9)	O9—H1W	0.82 (12)
C9—C10	1.555 (10)	O10—H3W	0.82 (5)
C10—O8	1.251 (8)	O10—H4W	0.82 (4)
C10—O7	1.287 (9)	O11—H6W	0.82 (4)
C11—O1	1.228 (7)	O11—H5W	0.82 (5)
O1—Ni1—O2^{i}	91.6 (2)	O1—C11—O2	124.2 (7)
O1—Ni1—O4^{i}	158.28 (17)	O1—C11—C12	119.4 (6)
O2^{i}—Ni1—O4^{i}	76.2 (2)	O2—C11—C12	116.3 (6)
O1—Ni1—O3	75.4 (2)	O3—C12—O4	128.8 (8)
O2^{i}—Ni1—O3	101.4 (2)	O3—C12—C11	114.9 (7)
O4^{i}—Ni1—O3	89.3 (2)	O4—C12—C11	116.3 (7)
O1—Ni1—N2	99.0 (2)	N1—C13—C14	123.2 (9)
O2^{i}—Ni1—N2	162.9 (2)	N1—C13—H13	118.4
O4^{i}—Ni1—N2	97.4 (2)	C14—C13—H13	118.4
O3—Ni1—N2	94.3 (2)	C15—C14—C13	118.2 (9)
O1—Ni1—N1	100.5 (2)	C15—C14—H14	120.9
O2^{i}—Ni1—N1	91.3 (2)	C13—C14—H14	120.9
O4^{i}—Ni1—N1	97.8 (2)	C16—C15—C14	121.9 (8)
O3—Ni1—N1	166.7 (2)	C16—C15—H15	119.0
N2—Ni1—N1	73.7 (2)	C14—C15—H15	119.1
O5^{ii}—Ni2—O6	91.0 (2)	C15—C16—C17	118.8 (9)
O5^{ii}—Ni2—O8	157.52 (16)	C15—C16—H16	120.6
O6—Ni2—O8	76.1 (2)	C17—C16—H16	120.6
O5^{ii}—Ni2—N5	100.1 (2)	N1—C17—C16	121.0 (8)
O6—Ni2—N5	162.0 (2)	N1—C17—C18	114.2 (7)
O8—Ni2—N5	97.3 (2)	C16—C17—C18	124.6 (8)
O5^{ii}—Ni2—O7^{ii}	76.95 (19)	N2—C18—C17	121.7 (7)
O6—Ni2—O7^{ii}	104.2 (2)	N2—C18—C19	107.2 (8)
O8—Ni2—O7^{ii}	88.3 (2)	C17—C18—C19	131.2 (8)
N5—Ni2—O7^{ii}	92.1 (2)	C20—C19—C18	106.3 (8)
O5^{ii}—Ni2—N4	99.5 (2)	C20—C19—H19	126.8
O6—Ni2—N4	91.5 (2)	C18—C19—H19	126.9
O8—Ni2—N4	99.2 (2)	C19—C20—N3	108.0 (9)
N5—Ni2—N4	72.9 (2)	C19—C20—H20	126.0
O7^{ii}—Ni2—N4	163.9 (2)	N3—C20—H20	126.0

N4—C1—C2	122.3 (8)	C13—N1—C17	116.6 (7)
N4—C1—H1	118.9	C13—N1—Ni1	127.5 (6)
C2—C1—H1	118.9	C17—N1—Ni1	115.8 (5)
C3—C2—C1	119.2 (9)	N3—N2—C18	108.4 (7)
C3—C2—H2	120.4	N3—N2—Ni1	136.9 (5)
C1—C2—H2	120.4	C18—N2—Ni1	114.3 (5)
C2—C3—C4	118.7 (8)	N2—N3—C20	109.9 (8)
C2—C3—H3	120.6	N2—N3—H3A	118 (3)
C4—C3—H3	120.6	C20—N3—H3A	132 (3)
C5—C4—C3	118.9 (9)	C5—N4—C1	118.6 (7)
C5—C4—H4	120.6	C5—N4—Ni2	115.7 (5)
C3—C4—H4	120.6	C1—N4—Ni2	125.6 (5)
N4—C5—C4	122.0 (9)	C6—N5—N6	102.3 (6)
N4—C5—C6	116.6 (7)	C6—N5—Ni2	119.1 (5)
C4—C5—C6	121.2 (8)	N6—N5—Ni2	138.5 (5)
N5—C6—C7	113.3 (8)	C8—N6—N5	111.7 (7)
N5—C6—C5	115.6 (7)	C8—N6—H6A	123 (10)
C7—C6—C5	131.1 (8)	N5—N6—H6A	116 (10)
C6—C7—C8	103.7 (8)	C11—O1—Ni1	114.3 (4)
C6—C7—H7	128.1	C11—O2—Ni1^{iii}	114.2 (5)
C8—C7—H7	128.1	C12—O3—Ni1	116.1 (6)
N6—C8—C7	108.9 (7)	C12—O4—Ni1^{iii}	116.1 (5)
N6—C8—H8	125.6	C9—O5—Ni2^{iv}	117.1 (4)
C7—C8—H8	125.6	C9—O6—Ni2	116.4 (6)
O6—C9—O5	128.1 (7)	C10—O7—Ni2^{iv}	111.8 (5)
O6—C9—C10	116.2 (7)	C10—O8—Ni2	113.6 (4)
O5—C9—C10	115.6 (6)	H2W—O9—H1W	116 (8)
O8—C10—O7	123.8 (8)	H3W—O10—H4W	115 (5)
O8—C10—C9	117.7 (6)	H6W—O11—H5W	114 (6)
O7—C10—C9	118.5 (6)		

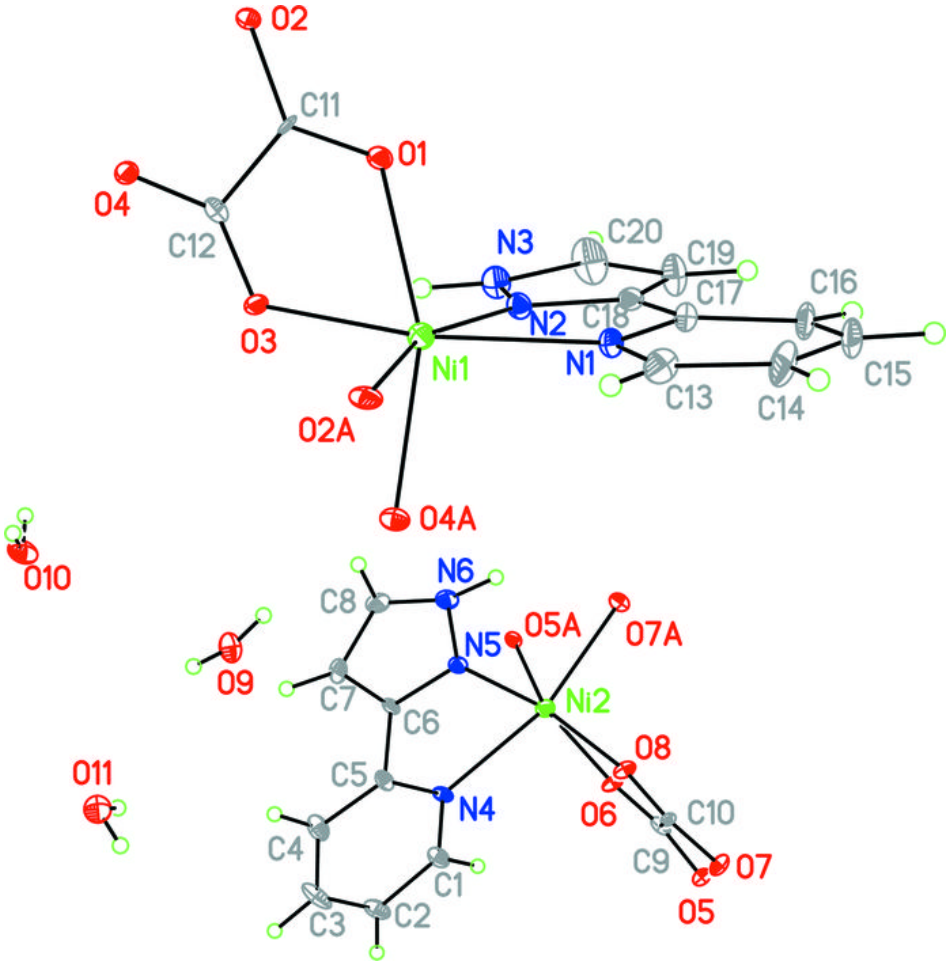
Symmetry codes: (i) *x*−1/2, −*y*+5/2, *z*; (ii) *x*+1/2, −*y*−1/2, *z*; (iii) *x*+1/2, −*y*+5/2, *z*; (iv) *x*−1/2, −*y*−1/2, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···O11^{v}	0.97 (4)	1.81 (2)	2.745 (10)	160 (5)
N6—H6A···O10^{vi}	0.98 (16)	2.0 (2)	2.732 (9)	133 (5)
O9—H2W···O7^{vii}	0.82 (4)	2.02 (4)	2.822 (9)	166 (6)
O9—H1W···O11^{viii}	0.82 (12)	2.22 (15)	2.813 (11)	130 (16)
O10—H3W···O4^{ix}	0.82 (5)	2.30 (7)	2.834 (9)	123 (7)
O10—H4W···O9^{viii}	0.82 (4)	2.08 (3)	2.811 (11)	148 (5)
O11—H5W···O9^{x}	0.82 (5)	2.15 (4)	2.813 (11)	138 (5)
O11—H6W···O8^{xi}	0.82 (4)	2.17 (4)	2.876 (9)	144 (6)

Symmetry codes: (v) −*x*+1, −*y*+2, *z*+1/2; (vi) *x*, *y*−1, *z*; (vii) *x*+1/2, −*y*+1/2, *z*; (viii) *x*+1/2, −*y*+3/2, *z*; (ix) −*x*+3/2, *y*−1/2, *z*−1/2; (x) *x*−1/2, −*y*+3/2, *z*; (xi) *x*, *y*+1, *z*.

Fig. 1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C11
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O4
C12
N3
C20
C19
C16
C17
C18
N2
O3
Ni1
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C15
C13
C14
O2A
O4A
O10
N6
C8
O5A
O7A
N5
O9
C7
Ni2
C6
O8
O11
C5
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O6
C10
C4
C9
O7
C1
O5
C3
C2

Fig. 2

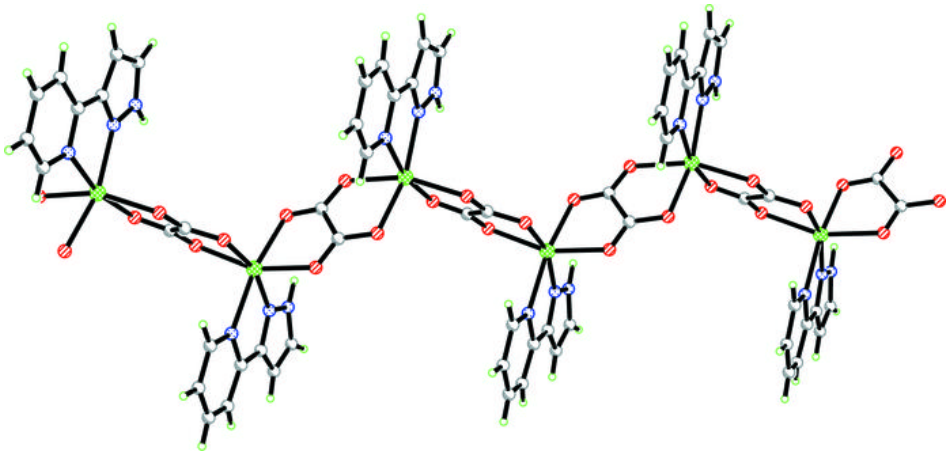

Fig. 3