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Crystal structure of poly[diaqua(μ_2-benzene-1,4-dicarboxylato-κ^2O^1:O^4)-(μ_2-benzene-1,4-dicarboxylato-$\kappa^4O^1,O^{1'}$:$O^4,O^{4'}$)bis(μ_2-3,3′,5,5′-tetramethyl-4,4′-bipyrazole-κ^2N:N')-dinickel(II)]

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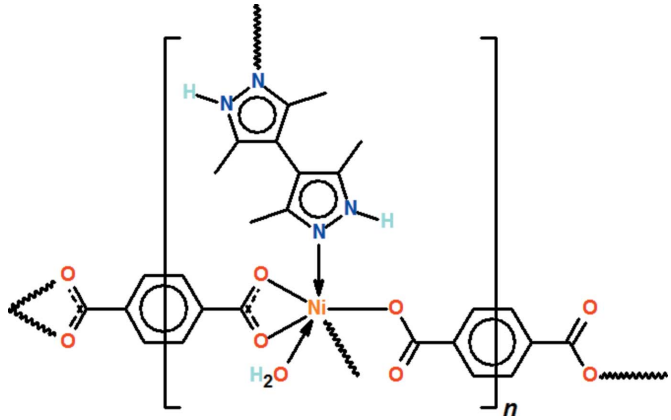
The asymmetric unit of the polymeric title compound, $[Ni(C_8H_4O_4)(C_{10}H_{14}N_4)(H_2O)]_n$, contains one Ni^{2+} cation, one coordinating water molecule, one 3,3′,5,5′-tetramethyl-4,4′-bipyrazole ligand and half each of two benzene-1,4-dicarboxylate anions, the other halves being generated by inversion symmetry. The Ni^{2+} cation exhibits an octahedral N_2O_4 coordination sphere defined by the O atoms of the water molecule and two different anions and the N atoms of two symmetry-related *N*-heterocycles. The *N*-heterocycles and both anions bridge adjacent Ni^{2+} cations into a three-dimensional network structure, with one of the anions in a bis-bidentate and the other in a bis-monodentate bridging mode. N—H···O and O—H···O hydrogen bonds between the N-heterocycles and water molecules as donor groups and the carboxylate O atoms as acceptor groups consolidate the crystal packing.

Keywords: crystal structure; nickel; coordination polymer; hydrogen bonding.

CCDC reference: 1062289

1. Related literature

In the related water-free coordination polymer {[Zn(terephthalate)(H_2Bpz)]·0.5(H_2Bpz)}$_n$ (H_2Bpz = 3,3′,5,5′-tetramethyl-4,4′-bipyrazole), the Zn^{2+} cation is tetrahedrally coordinated, see: He *et al.* (2007). For the structure of [Ni(terephthalate)-(pyrazole)$_4$], see: Hong *et al.* (2005).



2. Experimental

2.1. Crystal data

$[Ni(C_8H_4O_4)(C_{10}H_{14}N_4)(H_2O)]$
M_r = 431.09
Monoclinic, $P2_1/n$
a = 11.1603 (7) Å
b = 17.3367 (11) Å
c = 11.2345 (7) Å
β = 116.081 (1)°
V = 1952.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.03 mm^{-1}
T = 293 K
0.28 × 0.18 × 0.15 mm

2.2. Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
T_{min} = 0.645, T_{max} = 0.746
11758 measured reflections
4236 independent reflections
3627 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.098
S = 1.04
4236 reflections
272 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H11···O1^{i}	0.84 (1)	1.80 (2)	2.601 (2)	159 (4)
O1w—H12···O4^{i}	0.84 (1)	1.90 (2)	2.731 (2)	173 (3)
N2—H2···O4	0.88 (1)	1.98 (1)	2.837 (2)	164 (2)
N4—H4···O4^{ii}	0.87 (1)	2.23 (1)	3.080 (3)	164 (2)

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

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: WM5150).

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supporting information

Acta Cryst. (2015). E**71**, m127–m128 [doi:10.1107/S2056989015008415]

Crystal structure of poly[diaqua(μ_2-benzene-1,4-dicarboxylato-κ^2O^1:O^4)(μ_2-benzene-1,4-dicarboxylato-$\kappa^4O^1,O^{1'}$:$O^4,O^{4'}$)bis(μ_2-3,3′,5,5′-tetramethyl-4,4′-bipyrazole-κ^2N:N')dinickel(II)]

Chao Wu and Peng Cao

S1. Synthesis and crystallization

An aqueous mixture of nickel sulfate hexahydrate (52.6 mg, 0.2 mmol), 3,3′,5,5′-tetramethyl-4,4′-bipyrazole (38.1 mg, 0.2 mmol) and 1,4-benzene dicarboxylic acid (33.2 mg, 0.2 mmol) was placed in a Teflon-lined, stainless-steel reactor. The reactor was heated to 393 K for 48 hours. It was then cooled to room temperatuer at the rate of 5 K per hour. Green crystals were isolated in 70% yield. C, H, N elemental analysis. Calcd. for $C_{18}H_{20}N_4O_5Ni$: C 50.15, H 4.68, N 13.00%; found C 50.28, H 4.81, N 12.92%.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 to 0.96 Å) and were included in the refinement in the riding model approximation, with U(H) fixed at 1.2 to 1.5 times U_{iso}(C). The water and amino H-atoms were located in a difference Fourier map, and were refined with distance restraints of O—H 0.84 (1) Å and N—H 0.88 (1) Å; their U_{iso}(H) parameter were refined independently.

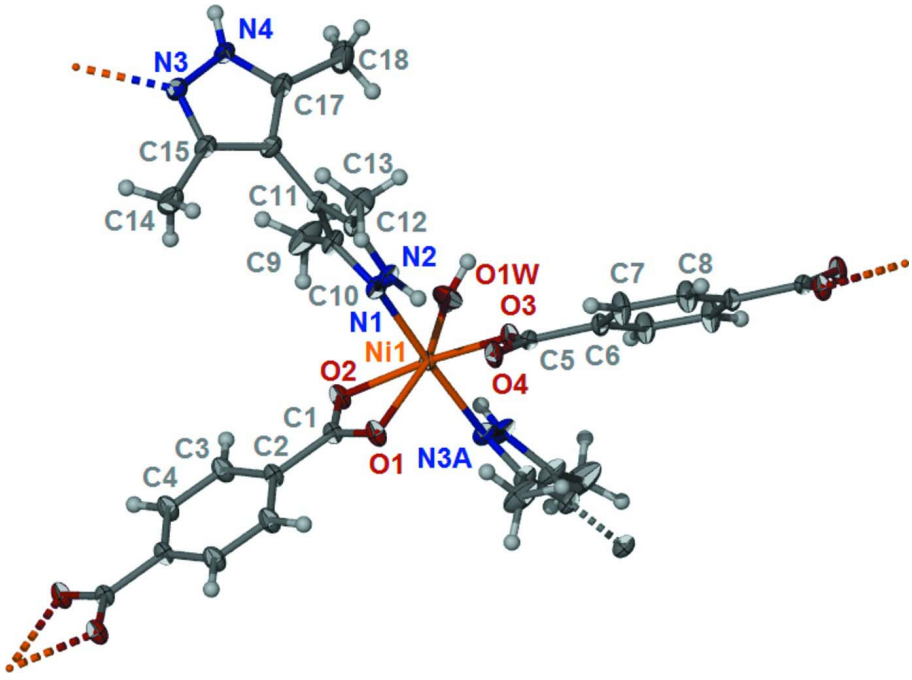

Figure 1

Displacement ellipsoid plot of a fragment of the three-dimensional network of $[Ni(H_2O)(C_{10}H_{14}N_4)(C_8H_4O_4)]_n$ drawn at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

Poly[diaqua(μ_2-benzene-1,4-dicarboxylato-κ^2O^1:O^4)(μ_2-benzene-1,4-dicarboxylato-κ^4O^1,$O^{1'}$:O^4,$O^{4'}$)bis(μ_2-3,3′,5,5′-tetramethyl-4,4′-bipyrazole-κ^2N:N')dinickel(II)]

Crystal data

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Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 11.1603 (7) Å
b = 17.3367 (11) Å
c = 11.2345 (7) Å
β = 116.081 (1)°
V = 1952.3 (2) Å^3
Z = 4
$F(000)$ = 896
D_x = 1.467 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3721 reflections
θ = 2.3–26.7°
μ = 1.03 mm^{-1}
T = 293 K
Prism, green
0.28 × 0.18 × 0.15 mm

Data collection

Bruker SMART diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
T_{min} = 0.645, T_{max} = 0.746
11758 measured reflections
4236 independent reflections
3627 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 27.0°, θ_{min} = 2.1°
h = −13→14
k = −21→22
l = −10→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.098$
$S = 1.04$
4236 reflections
272 parameters
4 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
$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.4664P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.36576 (2)	0.277787 (13)	0.18220 (2)	0.01814 (10)
O1	0.19348 (13)	0.32361 (8)	0.02675 (15)	0.0266 (3)
O2	0.29813 (13)	0.38770 (8)	0.21146 (14)	0.0261 (3)
O3	0.40583 (14)	0.17246 (8)	0.12360 (15)	0.0279 (3)
O4	0.21805 (14)	0.11750 (9)	−0.02559 (15)	0.0308 (4)
O1w	0.52381 (16)	0.27350 (9)	0.36205 (17)	0.0316 (4)
H11	0.561 (3)	0.2350 (13)	0.408 (3)	0.068 (11)*
H12	0.580 (2)	0.3083 (13)	0.400 (3)	0.057 (9)*
N1	0.24869 (18)	0.22143 (9)	0.25933 (18)	0.0253 (4)
N2	0.17275 (17)	0.15986 (10)	0.19515 (17)	0.0243 (4)
H2	0.172 (2)	0.1420 (14)	0.1219 (15)	0.034 (7)*
N3	−0.01548 (17)	0.17170 (10)	0.59896 (18)	0.0269 (4)
N4	0.10431 (19)	0.13770 (12)	0.67197 (19)	0.0326 (4)
H4	0.125 (3)	0.1247 (15)	0.7539 (13)	0.044 (8)*
C1	0.20219 (18)	0.38216 (11)	0.0984 (2)	0.0221 (4)
C2	0.09733 (19)	0.44350 (11)	0.0473 (2)	0.0234 (4)
C3	0.0975 (2)	0.50261 (12)	0.1296 (2)	0.0285 (5)
H3	0.1633	0.5043	0.2167	0.034*
C4	0.0006 (2)	0.55935 (12)	0.0835 (2)	0.0285 (5)
H4A	0.0007	0.5990	0.1393	0.034*
C5	0.3431 (2)	0.12127 (11)	0.0413 (2)	0.0241 (4)
C6	0.42497 (19)	0.05760 (12)	0.0211 (2)	0.0234 (4)
C7	0.3661 (2)	−0.01133 (13)	−0.0363 (3)	0.0348 (5)
H7	0.2760	−0.0193	−0.0602	0.042*
C8	0.4405 (2)	−0.06880 (13)	−0.0584 (2)	0.0326 (5)
H8	0.4000	−0.1148	−0.0983	0.039*
C9	0.2976 (3)	0.29163 (17)	0.4676 (3)	0.0512 (8)
H9A	0.3063	0.3368	0.4226	0.077*
H9B	0.3844	0.2748	0.5306	0.077*
H9C	0.2445	0.3036	0.5131	0.077*
C10	0.2318 (2)	0.22909 (12)	0.3692 (2)	0.0289 (5)
C11	0.1447 (2)	0.17158 (12)	0.3746 (2)	0.0262 (4)
C12	0.1100 (2)	0.12834 (12)	0.2614 (2)	0.0261 (4)

C13	0.0226 (2)	0.05878 (14)	0.2117 (3)	0.0408 (6)
H13A	−0.0315	0.0634	0.1180	0.061*
H13B	−0.0339	0.0549	0.2558	0.061*
H13C	0.0771	0.0134	0.2296	0.061*
C14	−0.1337 (3)	0.22052 (18)	0.3690 (3)	0.0508 (8)
H14A	−0.2020	0.2318	0.3964	0.076*
H14B	−0.1677	0.1850	0.2960	0.076*
H14C	−0.1066	0.2673	0.3419	0.076*
C15	−0.0169 (2)	0.18548 (13)	0.4814 (2)	0.0287 (5)
C16	0.1032 (2)	0.16093 (13)	0.4805 (2)	0.0278 (5)
C17	0.1780 (2)	0.13039 (15)	0.6040 (2)	0.0358 (5)
C18	0.3125 (3)	0.0935 (2)	0.6595 (3)	0.0668 (10)
H18A	0.3648	0.1117	0.7481	0.100*
H18B	0.3563	0.1065	0.6053	0.100*
H18C	0.3029	0.0385	0.6606	0.100*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01651 (14)	0.01908 (15)	0.01932 (16)	0.00261 (9)	0.00832 (11)	0.00007 (10)
O1	0.0223 (7)	0.0220 (7)	0.0284 (8)	0.0043 (5)	0.0047 (6)	−0.0059 (6)
O2	0.0222 (7)	0.0227 (7)	0.0269 (8)	0.0042 (5)	0.0049 (6)	−0.0023 (6)
O3	0.0311 (8)	0.0217 (7)	0.0331 (9)	0.0056 (6)	0.0161 (7)	−0.0049 (6)
O4	0.0239 (7)	0.0372 (9)	0.0292 (9)	0.0117 (6)	0.0097 (7)	−0.0029 (7)
O1w	0.0261 (8)	0.0268 (9)	0.0284 (9)	−0.0014 (6)	−0.0006 (7)	0.0042 (7)
N1	0.0289 (9)	0.0267 (9)	0.0251 (9)	−0.0038 (7)	0.0162 (8)	−0.0052 (7)
N2	0.0255 (8)	0.0302 (9)	0.0211 (9)	−0.0027 (7)	0.0138 (8)	−0.0041 (7)
N3	0.0248 (9)	0.0342 (10)	0.0237 (9)	0.0024 (7)	0.0126 (8)	0.0008 (8)
N4	0.0358 (10)	0.0439 (11)	0.0248 (11)	0.0133 (8)	0.0195 (9)	0.0087 (9)
C1	0.0194 (9)	0.0201 (10)	0.0258 (11)	0.0013 (7)	0.0090 (8)	0.0001 (8)
C2	0.0191 (9)	0.0208 (10)	0.0276 (11)	0.0029 (7)	0.0076 (8)	0.0001 (8)
C3	0.0241 (10)	0.0278 (11)	0.0249 (11)	0.0054 (8)	0.0027 (9)	−0.0024 (9)
C4	0.0295 (11)	0.0234 (10)	0.0265 (12)	0.0061 (8)	0.0069 (9)	−0.0043 (9)
C5	0.0293 (10)	0.0245 (10)	0.0231 (11)	0.0078 (8)	0.0158 (9)	0.0036 (8)
C6	0.0241 (10)	0.0238 (10)	0.0228 (11)	0.0064 (7)	0.0108 (8)	−0.0019 (8)
C7	0.0207 (10)	0.0328 (12)	0.0516 (15)	0.0008 (8)	0.0166 (10)	−0.0108 (11)
C8	0.0273 (11)	0.0262 (11)	0.0442 (14)	−0.0023 (8)	0.0157 (10)	−0.0132 (10)
C9	0.0678 (19)	0.0585 (17)	0.0416 (16)	−0.0270 (15)	0.0372 (15)	−0.0238 (13)
C10	0.0310 (11)	0.0344 (12)	0.0278 (12)	−0.0031 (9)	0.0190 (10)	−0.0045 (9)
C11	0.0266 (10)	0.0320 (11)	0.0251 (11)	0.0031 (8)	0.0159 (9)	0.0009 (9)
C12	0.0238 (10)	0.0306 (11)	0.0268 (11)	0.0009 (8)	0.0138 (9)	0.0009 (9)
C13	0.0405 (13)	0.0400 (14)	0.0455 (15)	−0.0118 (11)	0.0223 (12)	−0.0045 (11)
C14	0.0406 (15)	0.086 (2)	0.0278 (14)	0.0220 (14)	0.0174 (12)	0.0123 (14)
C15	0.0309 (11)	0.0345 (12)	0.0264 (12)	0.0011 (9)	0.0178 (10)	0.0006 (9)
C16	0.0293 (10)	0.0336 (12)	0.0261 (11)	0.0002 (9)	0.0173 (9)	0.0014 (9)
C17	0.0355 (12)	0.0491 (14)	0.0298 (13)	0.0106 (10)	0.0209 (11)	0.0032 (11)
C18	0.0548 (17)	0.109 (3)	0.0436 (17)	0.0446 (19)	0.0283 (14)	0.0177 (18)

Geometric parameters (Å, º)

Ni1—O1	2.1036 (14)	C5—C6	1.512 (3)
Ni1—O2	2.1276 (14)	C6—C7	1.380 (3)
Ni1—O3	2.0559 (14)	C6—C8^{iv}	1.383 (3)
Ni1—O1w	2.0164 (16)	C7—C8	1.388 (3)
Ni1—N1	2.0995 (17)	C7—H7	0.9300
Ni1—N3^{i}	2.1185 (17)	C8—C6^{iv}	1.383 (3)
O1—C1	1.273 (2)	C8—H8	0.9300
O2—C1	1.254 (2)	C9—C10	1.491 (3)
O3—C5	1.251 (3)	C9—H9A	0.9600
O4—C5	1.262 (2)	C9—H9B	0.9600
O1w—H11	0.836 (10)	C9—H9C	0.9600
O1w—H12	0.836 (10)	C10—C11	1.412 (3)
N1—C10	1.335 (3)	C11—C12	1.378 (3)
N1—N2	1.357 (2)	C11—C16	1.466 (3)
N2—C12	1.342 (3)	C12—C13	1.496 (3)
N2—H2	0.877 (10)	C13—H13A	0.9600
N3—C15	1.335 (3)	C13—H13B	0.9600
N3—N4	1.358 (2)	C13—H13C	0.9600
N3—Ni1^{ii}	2.1185 (17)	C14—C15	1.489 (3)
N4—C17	1.352 (3)	C14—H14A	0.9600
N4—H4	0.874 (10)	C14—H14B	0.9600
C1—C2	1.497 (3)	C14—H14C	0.9600
C2—C3	1.380 (3)	C15—C16	1.410 (3)
C2—C4^{iii}	1.395 (3)	C16—C17	1.372 (3)
C3—C4	1.383 (3)	C17—C18	1.493 (3)
C3—H3	0.9300	C18—H18A	0.9600
C4—C2^{iii}	1.395 (3)	C18—H18B	0.9600
C4—H4A	0.9300	C18—H18C	0.9600
O1w—Ni1—O3	94.04 (6)	C8^{iv}—C6—C5	119.95 (19)
O1w—Ni1—N1	89.90 (7)	C6—C7—C8	120.42 (19)
O3—Ni1—N1	88.93 (6)	C6—C7—H7	119.8
O1w—Ni1—O1	157.43 (6)	C8—C7—H7	119.8
O3—Ni1—O1	108.52 (6)	C6^{iv}—C8—C7	120.0 (2)
N1—Ni1—O1	90.63 (7)	C6^{iv}—C8—H8	120.0
O1w—Ni1—N3^{i}	90.92 (7)	C7—C8—H8	120.0
O3—Ni1—N3^{i}	87.68 (6)	C10—C9—H9A	109.5
N1—Ni1—N3^{i}	176.55 (7)	C10—C9—H9B	109.5
O1—Ni1—N3^{i}	89.90 (6)	H9A—C9—H9B	109.5
O1w—Ni1—O2	95.26 (6)	C10—C9—H9C	109.5
O3—Ni1—O2	170.69 (6)	H9A—C9—H9C	109.5
N1—Ni1—O2	91.47 (6)	H9B—C9—H9C	109.5
O1—Ni1—O2	62.17 (5)	N1—C10—C11	110.44 (19)
N3^{i}—Ni1—O2	91.79 (6)	N1—C10—C9	122.3 (2)
C1—O1—Ni1	89.33 (11)	C11—C10—C9	127.3 (2)
C1—O2—Ni1	88.74 (11)	C12—C11—C10	105.30 (18)

C5—O3—Ni1	137.48 (13)	C12—C11—C16	128.3 (2)
Ni1—O1w—H11	129 (2)	C10—C11—C16	126.3 (2)
Ni1—O1w—H12	127 (2)	N2—C12—C11	106.69 (18)
H11—O1w—H12	102 (3)	N2—C12—C13	122.4 (2)
C10—N1—N2	105.09 (17)	C11—C12—C13	130.9 (2)
C10—N1—Ni1	134.60 (15)	C12—C13—H13A	109.5
N2—N1—Ni1	120.24 (13)	C12—C13—H13B	109.5
C12—N2—N1	112.47 (17)	H13A—C13—H13B	109.5
C12—N2—H2	126.0 (16)	C12—C13—H13C	109.5
N1—N2—H2	121.4 (16)	H13A—C13—H13C	109.5
C15—N3—N4	104.79 (17)	H13B—C13—H13C	109.5
C15—N3—Ni1^{ii}	128.69 (15)	C15—C14—H14A	109.5
N4—N3—Ni1^{ii}	123.63 (14)	C15—C14—H14B	109.5
C17—N4—N3	112.41 (19)	H14A—C14—H14B	109.5
C17—N4—H4	128.6 (18)	C15—C14—H14C	109.5
N3—N4—H4	119.0 (17)	H14A—C14—H14C	109.5
O2—C1—O1	119.70 (17)	H14B—C14—H14C	109.5
O2—C1—C2	120.65 (18)	N3—C15—C16	110.80 (19)
O1—C1—C2	119.65 (18)	N3—C15—C14	122.5 (2)
C3—C2—C4^{iii}	120.16 (18)	C16—C15—C14	126.7 (2)
C3—C2—C1	120.00 (18)	C17—C16—C15	105.50 (19)
C4^{iii}—C2—C1	119.84 (18)	C17—C16—C11	126.9 (2)
C2—C3—C4	120.5 (2)	C15—C16—C11	127.4 (2)
C2—C3—H3	119.8	N4—C17—C16	106.5 (2)
C4—C3—H3	119.8	N4—C17—C18	123.6 (2)
C3—C4—C2^{iii}	119.38 (19)	C16—C17—C18	129.9 (2)
C3—C4—H4A	120.3	C17—C18—H18A	109.5
C2^{iii}—C4—H4A	120.3	C17—C18—H18B	109.5
O3—C5—O4	126.16 (18)	H18A—C18—H18B	109.5
O3—C5—C6	116.72 (18)	C17—C18—H18C	109.5
O4—C5—C6	117.12 (18)	H18A—C18—H18C	109.5
C7—C6—C8^{iv}	119.55 (19)	H18B—C18—H18C	109.5
C7—C6—C5	120.49 (18)		

O1w—Ni1—O1—C1	−1.3 (2)	Ni1—O3—C5—C6	170.67 (14)
O3—Ni1—O1—C1	178.98 (11)	O3—C5—C6—C7	161.3 (2)
N1—Ni1—O1—C1	89.91 (12)	O4—C5—C6—C7	−18.2 (3)
N3^{i}—Ni1—O1—C1	−93.50 (12)	O3—C5—C6—C8^{iv}	−19.8 (3)
O2—Ni1—O1—C1	−1.42 (11)	O4—C5—C6—C8^{iv}	160.8 (2)
O1w—Ni1—O2—C1	−178.52 (12)	C8^{iv}—C6—C7—C8	−0.9 (4)
O3—Ni1—O2—C1	3.8 (4)	C5—C6—C7—C8	178.0 (2)
N1—Ni1—O2—C1	−88.49 (12)	C6—C7—C8—C6^{iv}	0.9 (4)
O1—Ni1—O2—C1	1.45 (11)	N2—N1—C10—C11	0.2 (2)
N3^{i}—Ni1—O2—C1	90.39 (12)	Ni1—N1—C10—C11	−176.44 (15)
O1w—Ni1—O3—C5	157.3 (2)	N2—N1—C10—C9	−179.1 (2)
N1—Ni1—O3—C5	67.5 (2)	Ni1—N1—C10—C9	4.2 (4)
O1—Ni1—O3—C5	−22.8 (2)	N1—C10—C11—C12	0.2 (3)
N3^{i}—Ni1—O3—C5	−112.0 (2)	C9—C10—C11—C12	179.5 (3)

O2—Ni1—O3—C5	−25.1 (5)	N1—C10—C11—C16	179.4 (2)
O1w—Ni1—N1—C10	44.9 (2)	C9—C10—C11—C16	−1.3 (4)
O3—Ni1—N1—C10	138.9 (2)	N1—N2—C12—C11	0.7 (2)
O1—Ni1—N1—C10	−112.6 (2)	N1—N2—C12—C13	−178.74 (19)
N3^{i}—Ni1—N1—C10	148.7 (11)	C10—C11—C12—N2	−0.5 (2)
O2—Ni1—N1—C10	−50.4 (2)	C16—C11—C12—N2	−179.7 (2)
O1w—Ni1—N1—N2	−131.40 (15)	C10—C11—C12—C13	178.9 (2)
O3—Ni1—N1—N2	−37.35 (15)	C16—C11—C12—C13	−0.4 (4)
O1—Ni1—N1—N2	71.16 (15)	N4—N3—C15—C16	−0.7 (2)
N3^{i}—Ni1—N1—N2	−27.6 (12)	Ni1^{ii}—N3—C15—C16	160.26 (15)
O2—Ni1—N1—N2	133.34 (15)	N4—N3—C15—C14	178.0 (2)
C10—N1—N2—C12	−0.6 (2)	Ni1^{ii}—N3—C15—C14	−21.1 (3)
Ni1—N1—N2—C12	176.69 (14)	N3—C15—C16—C17	0.7 (3)
C15—N3—N4—C17	0.5 (3)	C14—C15—C16—C17	−177.9 (3)
Ni1^{ii}—N3—N4—C17	−161.73 (17)	N3—C15—C16—C11	−174.6 (2)
Ni1—O2—C1—O1	−2.43 (19)	C14—C15—C16—C11	6.8 (4)
Ni1—O2—C1—C2	177.19 (17)	C12—C11—C16—C17	103.9 (3)
Ni1—O1—C1—O2	2.46 (19)	C10—C11—C16—C17	−75.2 (3)
Ni1—O1—C1—C2	−177.17 (17)	C12—C11—C16—C15	−81.9 (3)
O2—C1—C2—C3	−7.0 (3)	C10—C11—C16—C15	99.1 (3)
O1—C1—C2—C3	172.62 (19)	N3—N4—C17—C16	0.0 (3)
O2—C1—C2—C4^{iii}	173.1 (2)	N3—N4—C17—C18	−178.6 (3)
O1—C1—C2—C4^{iii}	−7.2 (3)	C15—C16—C17—N4	−0.4 (3)
C4^{iii}—C2—C3—C4	0.2 (4)	C11—C16—C17—N4	174.9 (2)
C1—C2—C3—C4	−179.6 (2)	C15—C16—C17—C18	178.1 (3)
C2—C3—C4—C2^{iii}	−0.2 (4)	C11—C16—C17—C18	−6.6 (5)
Ni1—O3—C5—O4	−9.9 (4)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H11···O1^{v}	0.84 (1)	1.80 (2)	2.601 (2)	159 (4)
O1*w*—H12···O4^{v}	0.84 (1)	1.90 (2)	2.731 (2)	173 (3)
N2—H2···O4	0.88 (1)	1.98 (1)	2.837 (2)	164 (2)
N4—H4···O4^{vi}	0.87 (1)	2.23 (1)	3.080 (3)	164 (2)

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