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[3-Chloro-6-(3,5-dimethyl-1*H*-pyrazol-1-yl)picolinato](pyridine-2,6-dicarboxylato)nickel(II) dihydrate

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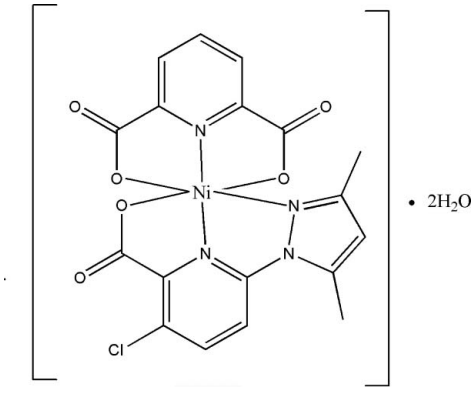
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.033; wR factor = 0.091; data-to-parameter ratio = 12.4.

In the title compound, $[Ni(C_{11}H_9ClN_3O_2)(C_7H_3NO_4)]\cdot 2H_2O$, the Ni^{II} atom is coordinated by two N atoms and one O atom of 3-chloro-6-(3,5-dimethyl-1*H*-pyrazol-1-yl)picolinate and by one N atom and two O atoms of pyridine-2,6-dicarboxylate in a distorted octahedral coordination. In the crystal structure, molecules are linked together by intermolecular O—H···O hydrogen bonds. One water molecule is disordered over two positions; the site occupancies are ca 0.53 and 0.47.

Related literature

For related literature, see: Bhatia *et al.* (1981); Costamagna *et al.* (1992).



Experimental

Crystal data

$[Ni(C_{11}H_9ClN_3O_2)(C_7H_3NO_4)]\cdot 2H_2O$
M_r = 510.51
Triclinic, $P\overline{1}$
a = 7.6267 (12) Å
b = 11.3464 (15) Å
c = 13.249 (2) Å
α = 109.607 (3)°
β = 91.782 (2)°
γ = 101.095 (2)°
V = 1054.2 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.10 mm^{-1}
T = 298 (2) K
0.58 × 0.45 × 0.44 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.568, T_{max} = 0.643
5476 measured reflections
3641 independent reflections
3129 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.091
S = 1.08
3641 reflections
293 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7D···O2	0.85	1.81	2.655 (3)	174
O7—H7E···O4^{i}	0.85	1.61	2.452 (3)	173
O8—H8A···O6	0.85	1.91	2.763 (6)	179
O8—H8B···O7^{ii}	0.85	1.77	2.623 (7)	179
O8′—H8′A···O6	0.85	1.90	2.751 (7)	180
O8′—H8′B···O7^{ii}	0.85	1.73	2.580 (7)	180

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: RK2060).

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[3-Chloro-6-(3,5-dimethyl-1*H*-pyrazol-1-yl)picolinato](pyridine-2,6-dicarboxylato)nickel(II) dihydrate

Yu Feng, Kai Zhao, Xian-Hong Yin, Jie Zhu and Cui-Wu Lin

S1. Comment

In recent years, there has been an increasing interest in the coordination chemistry due to the increased recognition of it's role in catalysis enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). We report here the crystal structure of a new nickel(II) complex with the ligand 3-chloro-6-(3,5-dimethyl-1*H*-pyrazol-1-yl) picolinic acid (CDPA) and pyridine-2,6-dicarboxylate (PDBL). (I) (Fig. 1).

The title compound, (I), consists of a central asymmetric Triclinic nickel(II) complex cation,two uncoordinated water molecules. In the cation (Fig. 1), the Ni atom is six-coordinated by three atoms and three O atoms from CDPA and PDBL ligands. The Ni(II) atom is a slightly distorted octahedral environment. The Ni—O bond length is 2.0699 (19), 2.0702 (18) and 2.2263 (18) Å, The Ni—N distances range from 1.973 (2) to 2.103 (2) Å, *i.e.* normal values. The C1—C2 bond length is 1.526 (3) Å, being in the normal C—C ranges in nickel carboxylate complexes. The angles around Ni(II) atom are from 76.78 (8) to 177.69 (8)°.

In the title compound, the oxygen atoms contribute to the formation of intermolecular hydrogen bonds involving water O atom. (Table 1 and Fig. 2).

S2. Experimental

3-chloro-(6-(3,5-dimethyl-1*H*-pyrazol-1-yl))picolinic acid, pyridine-2,6-dicarboxylic acid and $NiCl_2.6H_2O$ were available commercially and were used without further purification. Equimolar 3-chloro-6-(3,5-dimethyl-1*H*-pyrazol-1-yl)picolinic acid (0.5 mmol, 125 mg) and pyridine-2,6-dicarboxylic acid (0.5 mmol, 83 mg) were dissolved in anhydrous alcohol (15 ml). The mixture was stirred to give a clear solution, To this solution was added $NiCl_2.6H_2O$ (0.5 mmol, 113 mg) in anhydrous alcohol (10 ml). After keeping the resulting solution in air to evaporate about half of the solvents, dark red prisms of the title compound were formed. The crystals were isolated, washed with alcohol three times and dried in a vacuum desiccator using silica gel (Yield 75%). Elemental analysis: found: C, 42.25; H, 3.26; N, 10.88; O, 25.17; calc. for $C_{18}H_{16}Cl_{Ni}N_4O_8$: C, 42.35; H, 3.16; N, 10.98; O, 25.07.

S3. Refinement

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.93 Å and 0.96 Å for aromatic and methyl C atoms with U_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.5U_{eq}(C), respectively. One of two water molecules is disorder on two positions with ratio 0.531 (7)/0.469. The H atoms of water molecules were located from the difference Fourier map and constrained to ride on their parent atoms with O—H distances of 0.85 Å with and U_{iso}(H) = 1.2U_{eq}(O).

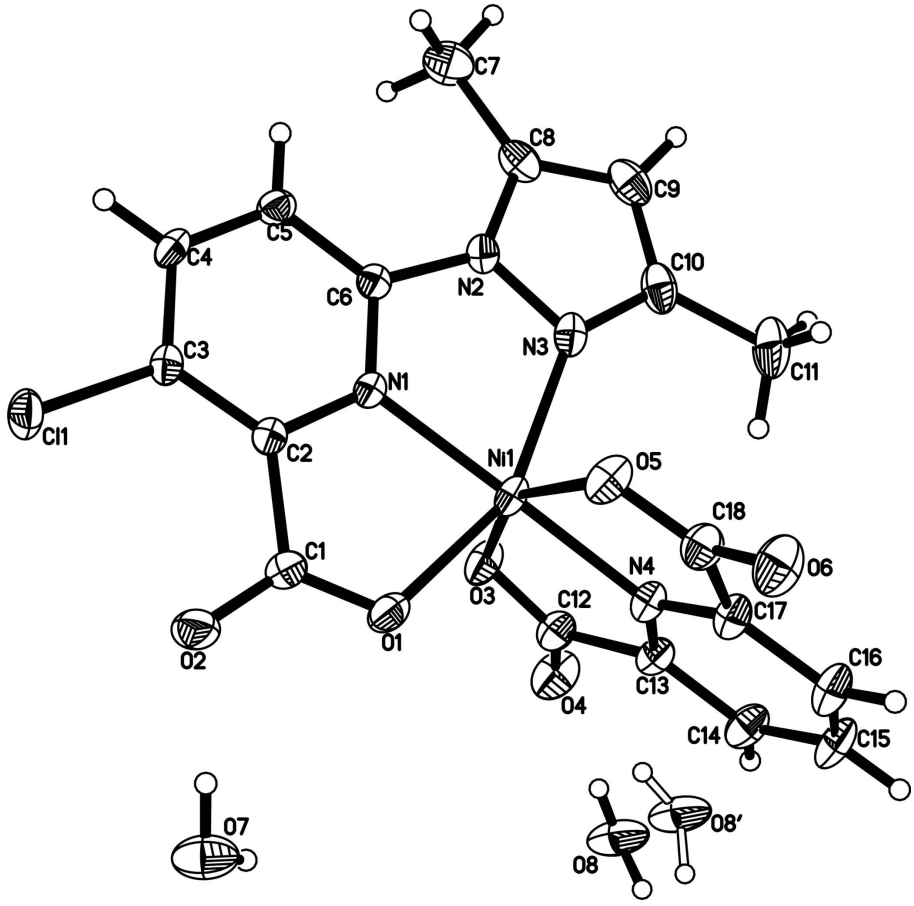

Figure 1

The structure of the title compound (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme.

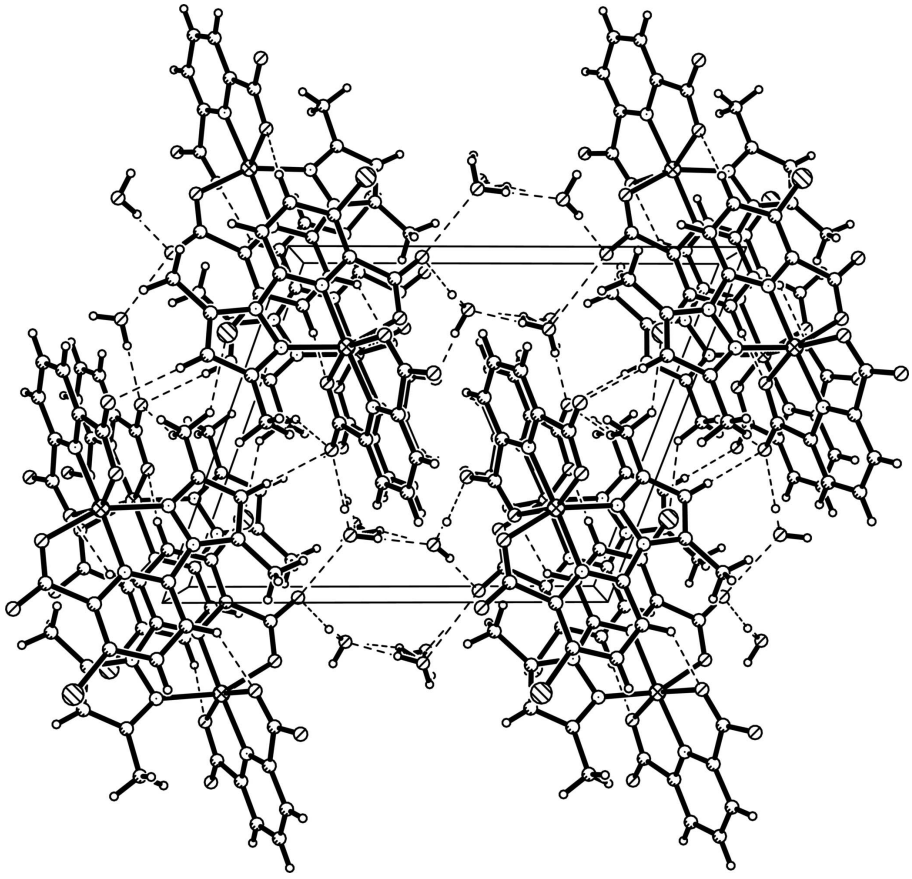

Figure 2

Crystal packing of (I) showing the hydrogen bonded interactions as dashed lines.

[3-Chloro-6-(3,5-dimethyl-1*H*-pyrazol-1-yl)picolinato](pyridine-2,6-dicarboxylato)nickel(II) dihydrate

Crystal data

$[Ni(C_{11}H_9ClN_3O_2)(C_7H_3NO_4)]\cdot 2H_2O$
$M_r = 510.51$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.6267\ (12)$ Å
$b = 11.3464\ (15)$ Å
$c = 13.249\ (2)$ Å
$\alpha = 109.607\ (3)°$
$\beta = 91.782\ (2)°$
$\gamma = 101.095\ (2)°$
$V = 1054.2\ (3)$ Å^3
$Z = 2$
$F(000) = 522$
$D_x = 1.608$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3593 reflections
$\theta = 2.7–28.1°$
$\mu = 1.10$ mm^{-1}
$T = 298$ K
Block, red
0.58 × 0.45 × 0.44 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.568$, $T_{max} = 0.643$
5476 measured reflections
3641 independent reflections
3129 reflections with $I > 2\sigma(I)$

R_{int} = 0.015
θ_{max} = 25.0°, θ_{min} = 2.0°
h = −9→9
k = −12→13
l = −15→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.091
S = 1.08
3641 reflections
293 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
$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 0.6077P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 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 $F^2 > 2\sigma(F^2)$ 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}	Occ. (<1)
Ni1	0.11832 (4)	0.72626 (3)	0.79837 (3)	0.03200 (12)	
Cl1	0.53279 (9)	1.22449 (6)	0.90615 (6)	0.04192 (18)	
N1	0.2169 (2)	0.90224 (17)	0.90552 (15)	0.0256 (4)	
N2	0.0633 (3)	0.83056 (19)	1.02607 (16)	0.0305 (5)	
N3	−0.0044 (3)	0.72177 (19)	0.93738 (18)	0.0340 (5)	
N4	0.0195 (3)	0.55626 (19)	0.68857 (17)	0.0324 (5)	
O1	0.2745 (3)	0.81200 (17)	0.70655 (14)	0.0430 (5)	
O2	0.4539 (3)	0.99224 (18)	0.71001 (16)	0.0490 (5)	
O3	−0.1242 (3)	0.75292 (17)	0.71801 (15)	0.0429 (5)	
O4	−0.3359 (3)	0.6456 (2)	0.57937 (18)	0.0534 (6)	
O5	0.3096 (2)	0.62668 (16)	0.81841 (15)	0.0421 (5)	
O6	0.3768 (3)	0.43402 (19)	0.75516 (18)	0.0538 (6)	
O7	0.6231 (3)	0.8470 (2)	0.56152 (17)	0.0604 (6)	
H7D	0.5680	0.8891	0.6113	0.073*	
H7E	0.6330	0.7786	0.5721	0.073*	
O8	0.4876 (11)	0.2126 (6)	0.6424 (5)	0.0688 (16)	0.531 (7)
H8A	0.4543	0.2808	0.6778	0.083*	0.531 (7)
H8B	0.4527	0.1929	0.5761	0.083*	0.531 (7)
O8′	0.3723 (12)	0.1814 (7)	0.6398 (6)	0.0688 (16)	0.469 (7)
H8′A	0.3732	0.2594	0.6753	0.083*	0.469 (7)
H8′B	0.3734	0.1723	0.5735	0.083*	0.469 (7)
C1	0.3524 (3)	0.9265 (2)	0.7521 (2)	0.0330 (6)	

C2	0.3239 (3)	0.9862 (2)	0.87041 (19)	0.0266 (5)
C3	0.3961 (3)	1.1083 (2)	0.9421 (2)	0.0279 (5)
C4	0.3575 (3)	1.1402 (2)	1.0492 (2)	0.0312 (5)
H4	0.4062	1.2217	1.0982	0.037*
C5	0.2487 (3)	1.0525 (2)	1.0825 (2)	0.0322 (5)
H5	0.2222	1.0730	1.1536	0.039*
C6	0.1791 (3)	0.9317 (2)	1.00644 (19)	0.0263 (5)
C7	0.0512 (5)	0.9129 (3)	1.2297 (2)	0.0551 (8)
H7A	−0.0074	0.8794	1.2804	0.083*
H7B	0.0150	0.9907	1.2337	0.083*
H7C	0.1790	0.9304	1.2464	0.083*
C8	−0.0002 (3)	0.8168 (3)	1.1183 (2)	0.0379 (6)
C9	−0.1110 (4)	0.6988 (3)	1.0864 (2)	0.0450 (7)
H9	−0.1753	0.6620	1.1308	0.054*
C10	−0.1108 (3)	0.6430 (3)	0.9752 (3)	0.0410 (7)
C11	−0.2136 (5)	0.5145 (3)	0.9029 (3)	0.0621 (9)
H11A	−0.3247	0.5233	0.8732	0.093*
H11B	−0.2381	0.4583	0.9435	0.093*
H11C	−0.1439	0.4794	0.8456	0.093*
C12	−0.2015 (4)	0.6548 (3)	0.6448 (2)	0.0388 (6)
C13	−0.1315 (4)	0.5346 (2)	0.6252 (2)	0.0371 (6)
C14	−0.2037 (4)	0.4148 (3)	0.5500 (2)	0.0472 (7)
H14	−0.3089	0.4001	0.5061	0.057*
C15	−0.1136 (4)	0.3176 (3)	0.5424 (2)	0.0507 (8)
H15	−0.1598	0.2354	0.4938	0.061*
C16	0.0447 (4)	0.3423 (3)	0.6069 (2)	0.0444 (7)
H16	0.1067	0.2777	0.6011	0.053*
C17	0.1093 (3)	0.4646 (2)	0.6802 (2)	0.0338 (6)
C18	0.2816 (4)	0.5107 (2)	0.7570 (2)	0.0367 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0352 (2)	0.02198 (18)	0.0315 (2)	0.00137 (13)	−0.00454 (13)	0.00317 (13)
Cl1	0.0429 (4)	0.0296 (3)	0.0491 (4)	−0.0041 (3)	0.0020 (3)	0.0152 (3)
N1	0.0259 (10)	0.0221 (9)	0.0269 (10)	0.0044 (8)	−0.0007 (8)	0.0067 (8)
N2	0.0267 (10)	0.0299 (10)	0.0330 (11)	0.0014 (8)	0.0001 (8)	0.0114 (9)
N3	0.0297 (11)	0.0275 (11)	0.0424 (13)	0.0007 (9)	−0.0021 (9)	0.0127 (9)
N4	0.0356 (11)	0.0258 (10)	0.0309 (11)	0.0027 (9)	−0.0042 (9)	0.0064 (9)
O1	0.0560 (12)	0.0331 (10)	0.0287 (10)	−0.0004 (9)	0.0038 (8)	0.0020 (8)
O2	0.0706 (14)	0.0365 (10)	0.0397 (11)	0.0088 (10)	0.0212 (10)	0.0133 (9)
O3	0.0491 (11)	0.0340 (10)	0.0396 (11)	0.0115 (9)	−0.0080 (9)	0.0045 (9)
O4	0.0479 (12)	0.0526 (12)	0.0547 (13)	0.0107 (10)	−0.0183 (10)	0.0143 (10)
O5	0.0400 (10)	0.0319 (10)	0.0439 (11)	0.0059 (8)	−0.0115 (8)	0.0020 (8)
O6	0.0575 (13)	0.0448 (11)	0.0565 (13)	0.0222 (10)	−0.0095 (10)	0.0095 (10)
O7	0.0828 (16)	0.0639 (14)	0.0482 (13)	0.0434 (13)	0.0183 (11)	0.0208 (11)
O8	0.125 (5)	0.054 (3)	0.0393 (15)	0.038 (4)	0.026 (4)	0.0198 (18)
O8′	0.125 (5)	0.054 (3)	0.0393 (15)	0.038 (4)	0.026 (4)	0.0198 (18)

C1	0.0389 (14)	0.0304 (13)	0.0285 (13)	0.0087 (11)	0.0026 (11)	0.0079 (11)
C2	0.0254 (12)	0.0248 (11)	0.0292 (13)	0.0060 (9)	0.0005 (10)	0.0087 (10)
C3	0.0242 (12)	0.0236 (11)	0.0349 (13)	0.0034 (9)	−0.0018 (10)	0.0102 (10)
C4	0.0319 (13)	0.0223 (11)	0.0313 (13)	0.0050 (10)	−0.0049 (10)	0.0001 (10)
C5	0.0322 (13)	0.0338 (13)	0.0264 (13)	0.0071 (11)	0.0011 (10)	0.0052 (10)
C6	0.0240 (12)	0.0269 (12)	0.0285 (13)	0.0070 (9)	0.0009 (9)	0.0096 (10)
C7	0.066 (2)	0.066 (2)	0.0377 (17)	0.0116 (17)	0.0136 (15)	0.0236 (15)
C8	0.0324 (14)	0.0488 (16)	0.0423 (15)	0.0122 (12)	0.0077 (11)	0.0261 (13)
C9	0.0386 (15)	0.0526 (17)	0.0578 (19)	0.0116 (13)	0.0130 (13)	0.0357 (15)
C10	0.0301 (14)	0.0351 (14)	0.0636 (19)	0.0043 (11)	0.0000 (12)	0.0267 (14)
C11	0.0520 (19)	0.0402 (17)	0.089 (3)	−0.0094 (14)	−0.0024 (18)	0.0270 (17)
C12	0.0379 (14)	0.0392 (15)	0.0368 (15)	0.0067 (12)	−0.0032 (12)	0.0117 (12)
C13	0.0390 (14)	0.0323 (13)	0.0342 (14)	0.0013 (11)	−0.0065 (11)	0.0086 (11)
C14	0.0498 (17)	0.0377 (15)	0.0416 (16)	−0.0027 (13)	−0.0157 (13)	0.0061 (12)
C15	0.065 (2)	0.0276 (14)	0.0418 (17)	−0.0026 (13)	−0.0135 (14)	−0.0016 (12)
C16	0.0595 (18)	0.0278 (13)	0.0404 (16)	0.0092 (12)	−0.0028 (13)	0.0058 (12)
C17	0.0416 (14)	0.0275 (12)	0.0292 (13)	0.0064 (11)	0.0000 (11)	0.0067 (10)
C18	0.0417 (15)	0.0324 (14)	0.0345 (14)	0.0080 (12)	−0.0020 (11)	0.0103 (11)

Geometric parameters (Å, º)

Ni1—N4	1.973 (2)	O8′—H8′A	0.8500
Ni1—N1	2.0052 (19)	O8′—H8′B	0.8500
Ni1—O1	2.0699 (19)	C1—C2	1.526 (3)
Ni1—O5	2.0702 (18)	C2—C3	1.384 (3)
Ni1—N3	2.103 (2)	C3—C4	1.398 (4)
Ni1—O3	2.2263 (18)	C4—C5	1.369 (4)
Cl1—C3	1.725 (2)	C4—H4	0.9300
N1—C6	1.321 (3)	C5—C6	1.392 (3)
N1—C2	1.346 (3)	C5—H5	0.9300
N2—C8	1.373 (3)	C7—C8	1.497 (4)
N2—N3	1.384 (3)	C7—H7A	0.9600
N2—C6	1.410 (3)	C7—H7B	0.9600
N3—C10	1.325 (3)	C7—H7C	0.9600
N4—C17	1.329 (3)	C8—C9	1.359 (4)
N4—C13	1.336 (3)	C9—C10	1.395 (4)
O1—C1	1.248 (3)	C9—H9	0.9300
O2—C1	1.245 (3)	C10—C11	1.494 (4)
O3—C12	1.231 (3)	C11—H11A	0.9600
O4—C12	1.286 (3)	C11—H11B	0.9600
O5—C18	1.266 (3)	C11—H11C	0.9600
O6—C18	1.231 (3)	C12—C13	1.506 (4)
O7—H7D	0.8500	C13—C14	1.382 (4)
O7—H7E	0.8500	C14—C15	1.386 (4)
O8—H8A	0.8500	C14—H14	0.9300
O8—H8B	0.8500	C15—C16	1.382 (4)
O8—H8′A	1.1315	C15—H15	0.9300
O8—H8′B	1.1478	C16—C17	1.384 (4)

O8′—H8A	1.1152	C16—H16	0.9300
O8′—H8B	1.0864	C17—C18	1.527 (4)
N4—Ni1—N1	177.69 (8)	C5—C4—C3	120.5 (2)
N4—Ni1—O1	99.98 (8)	C5—C4—H4	119.7
N1—Ni1—O1	78.32 (7)	C3—C4—H4	119.7
N4—Ni1—O5	79.21 (8)	C4—C5—C6	117.8 (2)
N1—Ni1—O5	102.38 (7)	C4—C5—H5	121.1
O1—Ni1—O5	92.69 (8)	C6—C5—H5	121.1
N4—Ni1—N3	104.83 (9)	N1—C6—C5	121.2 (2)
N1—Ni1—N3	76.78 (8)	N1—C6—N2	113.3 (2)
O1—Ni1—N3	154.97 (8)	C5—C6—N2	125.4 (2)
O5—Ni1—N3	95.02 (8)	C8—C7—H7A	109.5
N4—Ni1—O3	75.95 (8)	C8—C7—H7B	109.5
N1—Ni1—O3	102.36 (7)	H7A—C7—H7B	109.5
O1—Ni1—O3	88.72 (8)	C8—C7—H7C	109.5
O5—Ni1—O3	154.99 (7)	H7A—C7—H7C	109.5
N3—Ni1—O3	94.14 (8)	H7B—C7—H7C	109.5
C6—N1—C2	122.4 (2)	C9—C8—N2	105.7 (2)
C6—N1—Ni1	120.33 (15)	C9—C8—C7	128.8 (3)
C2—N1—Ni1	117.26 (16)	N2—C8—C7	125.5 (2)
C8—N2—N3	110.9 (2)	C8—C9—C10	107.7 (2)
C8—N2—C6	132.7 (2)	C8—C9—H9	126.2
N3—N2—C6	116.48 (19)	C10—C9—H9	126.2
C10—N3—N2	105.3 (2)	N3—C10—C9	110.4 (2)
C10—N3—Ni1	141.53 (19)	N3—C10—C11	121.8 (3)
N2—N3—Ni1	112.36 (14)	C9—C10—C11	127.8 (3)
C17—N4—C13	121.4 (2)	C10—C11—H11A	109.5
C17—N4—Ni1	117.36 (17)	C10—C11—H11B	109.5
C13—N4—Ni1	121.21 (17)	H11A—C11—H11B	109.5
C1—O1—Ni1	116.72 (16)	C10—C11—H11C	109.5
C12—O3—Ni1	112.55 (17)	H11A—C11—H11C	109.5
C18—O5—Ni1	115.55 (16)	H11B—C11—H11C	109.5
H7D—O7—H7E	108.5	O3—C12—O4	125.8 (3)
H8A—O8—H8B	108.4	O3—C12—C13	118.5 (2)
H8A—O8—H8′A	32.4	O4—C12—C13	115.6 (2)
H8B—O8—H8′A	96.6	N4—C13—C14	121.4 (2)
H8A—O8—H8′B	98.1	N4—C13—C12	111.6 (2)
H8B—O8—H8′B	30.6	C14—C13—C12	127.0 (2)
H8′A—O8—H8′B	74.4	C13—C14—C15	117.6 (3)
H8A—O8′—H8B	77.5	C13—C14—H14	121.2
H8A—O8′—H8′A	33.1	C15—C14—H14	121.2
H8B—O8′—H8′A	100.0	C16—C15—C14	120.2 (2)
H8A—O8′—H8′B	100.6	C16—C15—H15	119.9
H8B—O8′—H8′B	33.4	C14—C15—H15	119.9
H8′A—O8′—H8′B	108.4	C15—C16—C17	119.0 (3)
O2—C1—O1	125.5 (2)	C15—C16—H16	120.5
O2—C1—C2	118.7 (2)	C17—C16—H16	120.5

O1—C1—C2	115.8 (2)	N4—C17—C16	120.3 (2)
N1—C2—C3	119.1 (2)	N4—C17—C18	113.0 (2)
N1—C2—C1	111.90 (19)	C16—C17—C18	126.7 (2)
C3—C2—C1	129.0 (2)	O6—C18—O5	126.6 (2)
C2—C3—C4	119.0 (2)	O6—C18—C17	118.6 (2)
C2—C3—Cl1	123.27 (19)	O5—C18—C17	114.8 (2)
C4—C3—Cl1	117.74 (18)		

O1—Ni1—N1—C6	−177.34 (18)	N1—C2—C3—C4	0.9 (3)
O5—Ni1—N1—C6	−87.12 (18)	C1—C2—C3—C4	−176.9 (2)
N3—Ni1—N1—C6	5.20 (17)	N1—C2—C3—Cl1	−179.25 (17)
O3—Ni1—N1—C6	96.60 (17)	C1—C2—C3—Cl1	3.0 (3)
O1—Ni1—N1—C2	1.49 (16)	C2—C3—C4—C5	−0.6 (3)
O5—Ni1—N1—C2	91.70 (17)	Cl1—C3—C4—C5	179.48 (18)
N3—Ni1—N1—C2	−175.97 (18)	C3—C4—C5—C6	0.1 (4)
O3—Ni1—N1—C2	−84.57 (17)	C2—N1—C6—C5	0.1 (3)
C8—N2—N3—C10	0.9 (3)	Ni1—N1—C6—C5	178.85 (17)
C6—N2—N3—C10	−178.7 (2)	C2—N1—C6—N2	179.42 (19)
C8—N2—N3—Ni1	−171.27 (16)	Ni1—N1—C6—N2	−1.8 (3)
C6—N2—N3—Ni1	9.1 (2)	C4—C5—C6—N1	0.2 (3)
N4—Ni1—N3—C10	6.4 (3)	C4—C5—C6—N2	−179.1 (2)
N1—Ni1—N3—C10	−175.3 (3)	C8—N2—C6—N1	175.4 (2)
O1—Ni1—N3—C10	178.8 (2)	N3—N2—C6—N1	−5.2 (3)
O5—Ni1—N3—C10	−73.8 (3)	C8—N2—C6—C5	−5.3 (4)
O3—Ni1—N3—C10	83.0 (3)	N3—N2—C6—C5	174.1 (2)
N4—Ni1—N3—N2	174.29 (15)	N3—N2—C8—C9	−0.9 (3)
N1—Ni1—N3—N2	−7.43 (15)	C6—N2—C8—C9	178.6 (2)
O1—Ni1—N3—N2	−13.3 (3)	N3—N2—C8—C7	177.1 (3)
O5—Ni1—N3—N2	94.14 (15)	C6—N2—C8—C7	−3.4 (4)
O3—Ni1—N3—N2	−109.16 (15)	N2—C8—C9—C10	0.6 (3)
O1—Ni1—N4—C17	92.1 (2)	C7—C8—C9—C10	−177.4 (3)
O5—Ni1—N4—C17	1.28 (19)	N2—N3—C10—C9	−0.6 (3)
N3—Ni1—N4—C17	−91.1 (2)	Ni1—N3—C10—C9	167.8 (2)
O3—Ni1—N4—C17	178.3 (2)	N2—N3—C10—C11	178.6 (2)
O1—Ni1—N4—C13	−87.7 (2)	Ni1—N3—C10—C11	−13.0 (4)
O5—Ni1—N4—C13	−178.6 (2)	C8—C9—C10—N3	0.0 (3)
N3—Ni1—N4—C13	89.0 (2)	C8—C9—C10—C11	−179.1 (3)
O3—Ni1—N4—C13	−1.6 (2)	Ni1—O3—C12—O4	−174.0 (2)
N4—Ni1—O1—C1	176.92 (19)	Ni1—O3—C12—C13	3.5 (3)
N1—Ni1—O1—C1	−1.47 (19)	C17—N4—C13—C14	1.8 (4)
O5—Ni1—O1—C1	−103.56 (19)	Ni1—N4—C13—C14	−178.3 (2)
N3—Ni1—O1—C1	4.4 (3)	C17—N4—C13—C12	−176.2 (2)
O3—Ni1—O1—C1	101.42 (19)	Ni1—N4—C13—C12	3.7 (3)
N4—Ni1—O3—C12	−1.21 (19)	O3—C12—C13—N4	−4.7 (4)
N1—Ni1—O3—C12	177.16 (19)	O4—C12—C13—N4	173.0 (2)
O1—Ni1—O3—C12	99.4 (2)	O3—C12—C13—C14	177.4 (3)
O5—Ni1—O3—C12	5.8 (3)	O4—C12—C13—C14	−4.9 (4)
N3—Ni1—O3—C12	−105.5 (2)	N4—C13—C14—C15	−0.1 (5)

N4—Ni1—O5—C18	−0.09 (19)	C12—C13—C14—C15	177.6 (3)
N1—Ni1—O5—C18	−178.38 (19)	C13—C14—C15—C16	−1.4 (5)
O1—Ni1—O5—C18	−99.8 (2)	C14—C15—C16—C17	1.3 (5)
N3—Ni1—O5—C18	104.1 (2)	C13—N4—C17—C16	−1.9 (4)
O3—Ni1—O5—C18	−7.0 (3)	Ni1—N4—C17—C16	178.2 (2)
Ni1—O1—C1—O2	178.6 (2)	C13—N4—C17—C18	177.8 (2)
Ni1—O1—C1—C2	1.2 (3)	Ni1—N4—C17—C18	−2.1 (3)
C6—N1—C2—C3	−0.6 (3)	C15—C16—C17—N4	0.4 (4)
Ni1—N1—C2—C3	−179.41 (16)	C15—C16—C17—C18	−179.3 (3)
C6—N1—C2—C1	177.5 (2)	Ni1—O5—C18—O6	−179.8 (2)
Ni1—N1—C2—C1	−1.3 (2)	Ni1—O5—C18—C17	−0.9 (3)
O2—C1—C2—N1	−177.6 (2)	N4—C17—C18—O6	−179.1 (2)
O1—C1—C2—N1	0.0 (3)	C16—C17—C18—O6	0.6 (4)
O2—C1—C2—C3	0.3 (4)	N4—C17—C18—O5	2.0 (3)
O1—C1—C2—C3	177.9 (2)	C16—C17—C18—O5	−178.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7*D*···O2	0.85	1.81	2.655 (3)	174
O7—H7*E*···O4^{i}	0.85	1.61	2.452 (3)	173
O8—H8*A*···O6	0.85	1.91	2.763 (6)	179
O8—H8*B*···O7^{ii}	0.85	1.77	2.623 (7)	179
O8′—H8′*A*···O6	0.85	1.90	2.751 (7)	180
O8′—H8′*B*···O7^{ii}	0.85	1.73	2.580 (7)	180

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