Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetrakis[3-(2-pyridylamino)pyridine-κN]-nickel(II) diperchlorate ethanol disolvate

Zhi-Min Wang

College of Biology and Environment Engineering, Zhejiang Shuren University, Hangzhou 310015, People's Republic of China
Correspondence e-mail: hslj2004@126.com

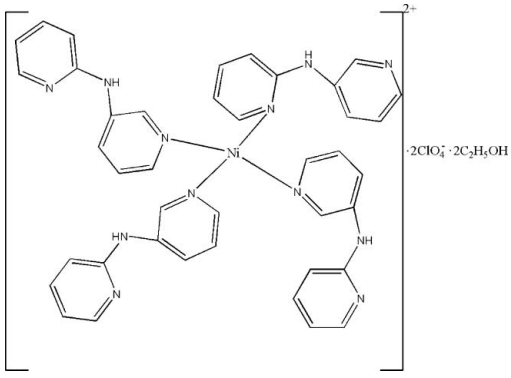
Received 7 March 2008; accepted 9 March 2008

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.048; wR factor = 0.135; data-to-parameter ratio = 13.7.

In the title compound, $[Ni(C_{10}H_9N_3)_4](ClO_4)_2\cdot 2C_2H_5OH$, the metal centre exhibits a four-coordinated environment with four pyridine N atoms of the four different dipyridylamine ligands. A twofold rotation axis passes through the Ni atom. N—H···O and N—H···N hydrogen bonds are present in the crystal structure.

Related literature

For related literature, see: Moulton & Zaworotko (2001); Su *et al.* (2003); Zhou *et al.* (2006); Biradha *et al.* (1999); Gudbjartson *et al.* (1999).



Experimental

Crystal data

$[Ni(C_{10}H_9N_3)_4](ClO_4)_2\cdot 2C_2H_6O$ M_r = 1034.55
Monoclinic, $C2/c$
a = 27.767 (4) Å
b = 10.7067 (14) Å
c = 18.144 (2) Å
β = 115.891 (9)°
V = 4852.6 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.58 mm^{-1}
T = 298 (2) K
0.32 × 0.22 × 0.17 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.836, T_{max} = 0.908
11042 measured reflections
4315 independent reflections
2875 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.134
S = 1.08
4315 reflections
314 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5B···O5	0.86	2.07	2.928 (5)	174
N2—H2···N6^{i}	0.86	2.27	3.129 (4)	176

Symmetry code: (i) $x, y-1, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The author is grateful to Shuren University for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2548).

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supporting information

Acta Cryst. (2008). E**64**, m540 [doi:10.1107/S1600536808006569]

Tetrakis[3-(2-pyridylamino)pyridine-κN]nickel(II) diperchlorate ethanol disolvate

Zhi-Min Wang

S1. Comment

In recent years, the rational design and assembly of metal-organic frameworks (MOFs) with well regulated network structures have received remarkable attention in order to develop new functional materials with potential applications (Moulton & Zaworotko, 2001). Nevertheless, it is still a great challenge to predict the exact structures and compositions of polymeric compounds assembled in a helical motif, although some structures with various helices have been reported in MOFs. So far, much of the research has been concentrated on the exploitation of angular ligands with a molecular angle, such as ligands with a T-shape, V-shape *etc*, in the construction of versatile coordination polymer architectures (Gudbjartson *et al.*, 1999; Su *et al.*, 2003, Zhou *et al.*, 2006). In this paper, we report the synthesis and crystal structure of the title complex with a V-shaped ligand,(I).

As shown in Fig. 1, the complex I is located twofold axis *via* the 2,3′-dipyridylamine (*L*) ligands. That I is a neutral, mononuclear molecule with the Ni(II) atom in a square coordination geometry with four pyridine nitrogen atoms of the four different *L* ligands. The Ni—N bond lengths range from 2.013 (2) to 2.019 (2)Å (Table1), and the N(1)—Ni—N(4) angle is 179.09 (11)°, it can be seen that the Ni(II) ions together with the four nitrogen atoms form a perfect square geometry, and this ideal quadrangle structure is rare in the coordination geometry of Ni(II) atom. Four *L* ligands present monodenate fashion. Two O atoms of the uncoordinated ClO_4 anions form the acceptors of intermolecular hydrogen bonds and weak interactions, which link the discrete units to form a two-dimensional supramolecular structure. The ethanol molecule present in I only functioned as an acceptor of intramolecular hydrogen bonds between the oxygen atoms of ethonal and amino nitrogen atoms of the ligand (Table 2), which stabilize the extended structure.

S2. Experimental

$NiClO_4$ (0.027 g, 0.013 mmol), *L* (0.025 g, 0.014 mmol) were added in a solvent of methanol, the mixture was heated for 6 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, Two weeks later some single crystals of the size suitable for X-Ray diffraction analysis.

S3. Refinement

The H atoms (pyridine ring) were placed in calculated positions [C—H = 0.93 - 0.97 Å and N—H = 0.86 Å] and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C,*N*) or 1.5U_{eq}(C_{methyl}).

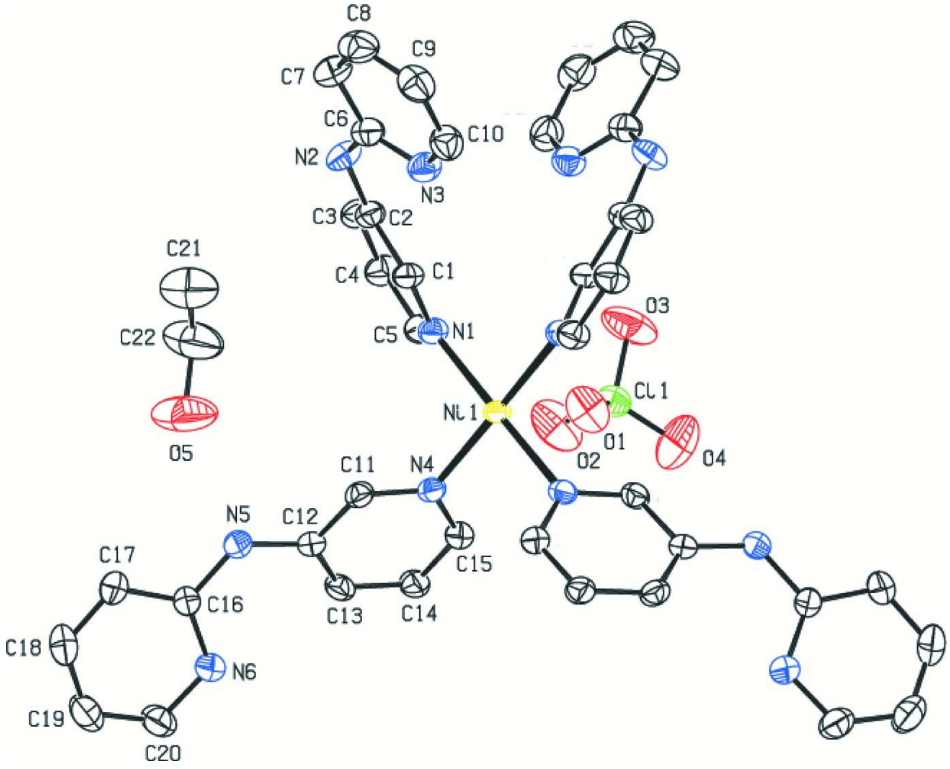

Figure 1

The asymmetric unit of (I), showing 30% probability displacement ellipsoids [symmetrical code: (i) -*x*, *y*, 1/2 - *z*].

Tetrakis[3-(2-pyridylamino)pyridine-*κN*]nickel(II) bis(perchlorate) ethanol disolvate

Crystal data

$[Ni(C_{10}H_9N_3)_4](ClO_4)_2\cdot 2C_2H_6O$
$M_r = 1034.55$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 27.767\ (4)$ Å
$b = 10.7067\ (14)$ Å
$c = 18.144\ (2)$ Å
$\beta = 115.891\ (9)°$
$V = 4852.6\ (11)$ Å^3
$Z = 4$
$F(000) = 2152$
$D_x = 1.416$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4315 reflections
$\theta = 1.6–25.1°$
$\mu = 0.58$ mm^{-1}
$T = 298$ K
Block, green
0.32 × 0.22 × 0.17 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.836$, $T_{max} = 0.908$
11042 measured reflections
4315 independent reflections
2875 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 25.1°$, $\theta_{min} = 1.6°$
$h = -33\rightarrow33$
$k = -12\rightarrow12$
$l = -21\rightarrow21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.134$
$S = 1.08$
4315 reflections
314 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
$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 1.1196P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.084$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ 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 $F^2 > \sigma(F^2)$ 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}
Ni1	0.5000	0.23720 (5)	0.7500	0.0397 (2)
N1	0.54118 (10)	0.1032 (2)	0.72421 (16)	0.0455 (6)
N2	0.60983 (11)	−0.1938 (3)	0.80972 (17)	0.0586 (8)
H2	0.6337	−0.2349	0.8016	0.070*
N3	0.56191 (11)	−0.1786 (3)	0.88745 (18)	0.0577 (7)
N4	0.54239 (10)	0.3700 (2)	0.72509 (16)	0.0438 (6)
N5	0.68140 (10)	0.4606 (3)	0.79766 (17)	0.0550 (7)
H5B	0.6945	0.3923	0.8237	0.066*
N6	0.69860 (11)	0.6684 (3)	0.77848 (18)	0.0574 (7)
C1	0.56303 (12)	0.0085 (3)	0.77601 (19)	0.0456 (8)
H1	0.5621	0.0104	0.8267	0.055*
C2	0.58706 (13)	−0.0930 (3)	0.7574 (2)	0.0474 (8)
C3	0.58891 (14)	−0.0912 (3)	0.6822 (2)	0.0547 (9)
H3	0.6051	−0.1566	0.6677	0.066*
C4	0.56711 (14)	0.0061 (3)	0.6297 (2)	0.0565 (9)
H4	0.5684	0.0073	0.5794	0.068*
C5	0.54302 (13)	0.1029 (3)	0.6514 (2)	0.0515 (8)
H5	0.5279	0.1687	0.6152	0.062*
C6	0.59913 (15)	−0.2364 (3)	0.8729 (2)	0.0544 (9)
C7	0.62701 (16)	−0.3403 (4)	0.9173 (2)	0.0682 (11)
H7	0.6529	−0.3791	0.9058	0.082*
C8	0.61504 (17)	−0.3838 (4)	0.9787 (2)	0.0757 (11)
H8	0.6324	−0.4540	1.0089	0.091*
C9	0.57742 (17)	−0.3231 (4)	0.9951 (2)	0.0720 (11)
H9	0.5692	−0.3502	1.0369	0.086*

C10	0.55247 (15)	−0.2224 (4)	0.9489 (2)	0.0643 (10)
H10	0.5272	−0.1812	0.9606	0.077*
C11	0.59564 (12)	0.3773 (3)	0.76688 (19)	0.0437 (7)
H11	0.6127	0.3229	0.8106	0.052*
C12	0.62665 (12)	0.4614 (3)	0.74861 (19)	0.0426 (7)
C13	0.60115 (12)	0.5367 (3)	0.6812 (2)	0.0477 (8)
H13	0.6208	0.5904	0.6645	0.057*
C14	0.54629 (13)	0.5316 (3)	0.6387 (2)	0.0525 (8)
H14	0.5285	0.5841	0.5942	0.063*
C15	0.51777 (13)	0.4489 (3)	0.6622 (2)	0.0515 (8)
H15	0.4806	0.4475	0.6339	0.062*
C16	0.71742 (12)	0.5563 (3)	0.8097 (2)	0.0480 (8)
C17	0.77153 (13)	0.5330 (4)	0.8563 (2)	0.0653 (10)
H17	0.7835	0.4542	0.8784	0.078*
C18	0.80698 (16)	0.6289 (5)	0.8690 (3)	0.0827 (13)
H18	0.8434	0.6163	0.9007	0.099*
C19	0.78839 (18)	0.7437 (4)	0.8349 (3)	0.0815 (13)
H19	0.8118	0.8094	0.8415	0.098*
C20	0.73503 (16)	0.7584 (4)	0.7913 (3)	0.0701 (11)
H20	0.7226	0.8366	0.7686	0.084*
Cl1	0.39899 (4)	0.22782 (8)	0.51603 (5)	0.0580 (3)
O1	0.42456 (13)	0.2385 (3)	0.60132 (16)	0.0903 (10)
O2	0.43498 (15)	0.2706 (3)	0.4854 (2)	0.1180 (13)
O3	0.38628 (16)	0.1017 (3)	0.4956 (2)	0.1268 (14)
O4	0.35263 (17)	0.2973 (5)	0.4863 (4)	0.196 (2)
O5	0.7269 (3)	0.2376 (3)	0.8974 (3)	0.166 (2)
H5A	0.7075	0.2571	0.9190	0.249*
C21	0.7270 (3)	0.0252 (6)	0.9344 (4)	0.143 (2)
H21A	0.7532	0.0553	0.9863	0.215*
H21B	0.7396	−0.0506	0.9206	0.215*
H21C	0.6940	0.0094	0.9378	0.215*
C22	0.7186 (3)	0.1150 (6)	0.8741 (4)	0.151 (3)
H22A	0.7416	0.0948	0.8482	0.181*
H22B	0.6819	0.1068	0.8327	0.181*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0470 (3)	0.0271 (3)	0.0562 (4)	0.000	0.0329 (3)	0.000
N1	0.0539 (16)	0.0367 (15)	0.0564 (16)	0.0018 (12)	0.0340 (14)	0.0022 (13)
N2	0.070 (2)	0.0493 (17)	0.0644 (19)	0.0226 (15)	0.0365 (17)	0.0081 (15)
N3	0.0660 (19)	0.0489 (18)	0.0645 (19)	0.0046 (14)	0.0344 (17)	0.0068 (15)
N4	0.0470 (16)	0.0328 (14)	0.0556 (16)	0.0043 (12)	0.0261 (14)	0.0038 (13)
N5	0.0428 (16)	0.0420 (16)	0.071 (2)	0.0045 (12)	0.0166 (15)	0.0154 (14)
N6	0.0506 (17)	0.0438 (18)	0.073 (2)	−0.0016 (14)	0.0221 (16)	0.0044 (15)
C1	0.057 (2)	0.0342 (17)	0.0531 (19)	0.0017 (15)	0.0311 (17)	0.0019 (16)
C2	0.0508 (19)	0.0390 (18)	0.058 (2)	0.0035 (15)	0.0285 (17)	−0.0007 (16)
C3	0.065 (2)	0.046 (2)	0.064 (2)	0.0063 (17)	0.0384 (19)	−0.0056 (18)

C4	0.072 (2)	0.052 (2)	0.059 (2)	0.0061 (18)	0.041 (2)	0.0009 (18)
C5	0.063 (2)	0.046 (2)	0.058 (2)	0.0033 (16)	0.0376 (18)	0.0063 (17)
C6	0.061 (2)	0.044 (2)	0.054 (2)	0.0017 (17)	0.0212 (18)	−0.0013 (17)
C7	0.079 (3)	0.054 (2)	0.068 (3)	0.017 (2)	0.029 (2)	0.011 (2)
C8	0.086 (3)	0.056 (3)	0.065 (3)	0.003 (2)	0.014 (2)	0.012 (2)
C9	0.075 (3)	0.075 (3)	0.059 (2)	−0.012 (2)	0.023 (2)	0.014 (2)
C10	0.061 (2)	0.069 (3)	0.065 (2)	−0.0037 (19)	0.029 (2)	0.006 (2)
C11	0.045 (2)	0.0372 (18)	0.0494 (19)	0.0069 (14)	0.0213 (16)	0.0081 (15)
C12	0.0455 (18)	0.0325 (16)	0.0498 (18)	0.0019 (13)	0.0208 (16)	0.0001 (14)
C13	0.051 (2)	0.0383 (18)	0.054 (2)	−0.0073 (15)	0.0230 (17)	0.0052 (16)
C14	0.048 (2)	0.0414 (19)	0.057 (2)	−0.0002 (15)	0.0123 (17)	0.0124 (16)
C15	0.0446 (19)	0.0412 (19)	0.063 (2)	−0.0004 (15)	0.0184 (17)	0.0032 (17)
C16	0.0405 (18)	0.047 (2)	0.056 (2)	−0.0021 (15)	0.0204 (16)	−0.0038 (16)
C17	0.043 (2)	0.061 (2)	0.079 (3)	0.0068 (17)	0.0141 (19)	0.003 (2)
C18	0.043 (2)	0.095 (4)	0.101 (3)	−0.008 (2)	0.024 (2)	−0.006 (3)
C19	0.064 (3)	0.077 (3)	0.096 (3)	−0.026 (2)	0.029 (3)	−0.005 (3)
C20	0.067 (3)	0.054 (2)	0.078 (3)	−0.0135 (19)	0.022 (2)	0.006 (2)
Cl1	0.0655 (6)	0.0541 (6)	0.0529 (5)	−0.0062 (4)	0.0243 (5)	−0.0040 (4)
O1	0.104 (2)	0.120 (3)	0.0521 (16)	−0.0282 (18)	0.0392 (17)	−0.0173 (15)
O2	0.150 (3)	0.146 (3)	0.084 (2)	−0.053 (2)	0.076 (2)	0.000 (2)
O3	0.183 (4)	0.082 (2)	0.152 (3)	−0.060 (2)	0.106 (3)	−0.062 (2)
O4	0.095 (3)	0.162 (4)	0.274 (6)	0.057 (3)	0.026 (4)	0.053 (4)
O5	0.221 (6)	0.067 (2)	0.128 (4)	0.010 (3)	0.001 (3)	0.019 (2)
C21	0.189 (7)	0.092 (4)	0.147 (6)	−0.001 (4)	0.072 (5)	0.004 (4)
C22	0.187 (7)	0.080 (4)	0.129 (5)	−0.028 (4)	0.017 (5)	0.013 (4)

Geometric parameters (Å, º)

Ni1—N1^{i}	2.013 (2)	C9—C10	1.356 (5)
Ni1—N1	2.013 (2)	C9—H9	0.9300
Ni1—N4	2.019 (2)	C10—H10	0.9300
Ni1—N4^{i}	2.019 (2)	C11—C12	1.382 (4)
N1—C1	1.335 (4)	C11—H11	0.9300
N1—C5	1.344 (4)	C12—C13	1.375 (4)
N2—C6	1.382 (4)	C13—C14	1.375 (4)
N2—C2	1.393 (4)	C13—H13	0.9300
N2—H2	0.8600	C14—C15	1.373 (4)
N3—C6	1.326 (4)	C14—H14	0.9300
N3—C10	1.336 (4)	C15—H15	0.9300
N4—C11	1.337 (4)	C16—C17	1.388 (5)
N4—C15	1.342 (4)	C17—C18	1.371 (5)
N5—C16	1.381 (4)	C17—H17	0.9300
N5—C12	1.386 (4)	C18—C19	1.371 (6)
N5—H5B	0.8600	C18—H18	0.9300
N6—C16	1.332 (4)	C19—C20	1.350 (6)
N6—C20	1.342 (4)	C19—H19	0.9300
C1—C2	1.392 (4)	C20—H20	0.9300
C1—H1	0.9300	Cl1—O4	1.377 (4)

C2—C3	1.388 (4)	Cl1—O1	1.397 (3)
C3—C4	1.362 (5)	Cl1—O3	1.404 (3)
C3—H3	0.9300	Cl1—O2	1.415 (3)
C4—C5	1.381 (4)	O5—C22	1.368 (6)
C4—H4	0.9300	O5—H5A	0.8200
C5—H5	0.9300	C21—C22	1.397 (7)
C6—C7	1.394 (5)	C21—H21A	0.9600
C7—C8	1.376 (5)	C21—H21B	0.9600
C7—H7	0.9300	C21—H21C	0.9600
C8—C9	1.369 (5)	C22—H22A	0.9700
C8—H8	0.9300	C22—H22B	0.9700

$N1^{i}$—Ni1—N1	89.08 (14)	N4—C11—C12	123.5 (3)
$N1^{i}$—Ni1—N4	179.09 (11)	N4—C11—H11	118.2
N1—Ni1—N4	90.24 (10)	C12—C11—H11	118.2
$N1^{i}$—Ni1—$N4^{i}$	90.24 (10)	C13—C12—C11	117.5 (3)
N1—Ni1—$N4^{i}$	179.09 (11)	C13—C12—N5	124.7 (3)
N4—Ni1—$N4^{i}$	90.44 (13)	C11—C12—N5	117.7 (3)
C1—N1—C5	119.3 (3)	C12—C13—C14	119.3 (3)
C1—N1—Ni1	120.49 (19)	C12—C13—H13	120.4
C5—N1—Ni1	120.0 (2)	C14—C13—H13	120.4
C6—N2—C2	128.5 (3)	C15—C14—C13	120.0 (3)
C6—N2—H2	115.7	C15—C14—H14	120.0
C2—N2—H2	115.7	C13—C14—H14	120.0
C6—N3—C10	117.1 (3)	N4—C15—C14	121.4 (3)
C11—N4—C15	118.2 (3)	N4—C15—H15	119.3
C11—N4—Ni1	121.5 (2)	C14—C15—H15	119.3
C15—N4—Ni1	120.2 (2)	N6—C16—N5	118.6 (3)
C16—N5—C12	127.8 (3)	N6—C16—C17	122.7 (3)
C16—N5—H5B	116.1	N5—C16—C17	118.7 (3)
C12—N5—H5B	116.1	C18—C17—C16	118.4 (4)
C16—N6—C20	116.6 (3)	C18—C17—H17	120.8
N1—C1—C2	122.8 (3)	C16—C17—H17	120.8
N1—C1—H1	118.6	C17—C18—C19	119.6 (4)
C2—C1—H1	118.6	C17—C18—H18	120.2
C3—C2—C1	117.0 (3)	C19—C18—H18	120.2
C3—C2—N2	118.7 (3)	C20—C19—C18	118.0 (4)
C1—C2—N2	124.3 (3)	C20—C19—H19	121.0
C4—C3—C2	120.2 (3)	C18—C19—H19	121.0
C4—C3—H3	119.9	N6—C20—C19	124.7 (4)
C2—C3—H3	119.9	N6—C20—H20	117.7
C3—C4—C5	119.8 (3)	C19—C20—H20	117.7
C3—C4—H4	120.1	O4—Cl1—O1	109.0 (3)
C5—C4—H4	120.1	O4—Cl1—O3	109.4 (3)
N1—C5—C4	120.9 (3)	O1—Cl1—O3	108.6 (2)
N1—C5—H5	119.6	O4—Cl1—O2	111.8 (3)
C4—C5—H5	119.6	O1—Cl1—O2	107.7 (2)
N3—C6—N2	118.7 (3)	O3—Cl1—O2	110.3 (2)

N3—C6—C7	122.8 (3)	C22—O5—H5A	109.5
N2—C6—C7	118.5 (3)	C22—C21—H21A	109.5
C8—C7—C6	118.0 (4)	C22—C21—H21B	109.5
C8—C7—H7	121.0	H21A—C21—H21B	109.5
C6—C7—H7	121.0	C22—C21—H21C	109.5
C9—C8—C7	119.5 (4)	H21A—C21—H21C	109.5
C9—C8—H8	120.3	H21B—C21—H21C	109.5
C7—C8—H8	120.3	O5—C22—C21	118.1 (6)
C10—C9—C8	118.4 (4)	O5—C22—H22A	107.8
C10—C9—H9	120.8	C21—C22—H22A	107.8
C8—C9—H9	120.8	O5—C22—H22B	107.8
N3—C10—C9	124.2 (4)	C21—C22—H22B	107.8
N3—C10—H10	117.9	H22A—C22—H22B	107.1
C9—C10—H10	117.9		

N1^{i}—Ni1—N1—C1	−48.8 (2)	C6—C7—C8—C9	−1.2 (6)
N4—Ni1—N1—C1	130.6 (2)	C7—C8—C9—C10	1.0 (6)
N1^{i}—Ni1—N1—C5	125.6 (3)	C6—N3—C10—C9	−1.8 (6)
N4—Ni1—N1—C5	−55.0 (3)	C8—C9—C10—N3	0.5 (6)
N1—Ni1—N4—C11	−59.8 (2)	C15—N4—C11—C12	−0.2 (4)
N4^{i}—Ni1—N4—C11	120.8 (3)	Ni1—N4—C11—C12	175.7 (2)
N1—Ni1—N4—C15	116.0 (2)	N4—C11—C12—C13	−3.4 (4)
N4^{i}—Ni1—N4—C15	−63.4 (2)	N4—C11—C12—N5	179.0 (3)
C5—N1—C1—C2	−1.2 (5)	C16—N5—C12—C13	25.5 (5)
Ni1—N1—C1—C2	173.2 (2)	C16—N5—C12—C11	−157.0 (3)
N1—C1—C2—C3	1.7 (5)	C11—C12—C13—C14	4.5 (4)
N1—C1—C2—N2	−179.5 (3)	N5—C12—C13—C14	−178.0 (3)
C6—N2—C2—C3	−157.8 (3)	C12—C13—C14—C15	−2.2 (5)
C6—N2—C2—C1	23.3 (6)	C11—N4—C15—C14	2.7 (4)
C1—C2—C3—C4	−0.9 (5)	Ni1—N4—C15—C14	−173.3 (2)
N2—C2—C3—C4	−179.9 (3)	C13—C14—C15—N4	−1.5 (5)
C2—C3—C4—C5	−0.2 (5)	C20—N6—C16—N5	−179.7 (3)
C1—N1—C5—C4	0.0 (5)	C20—N6—C16—C17	2.8 (5)
Ni1—N1—C5—C4	−174.4 (2)	C12—N5—C16—N6	7.6 (5)
C3—C4—C5—N1	0.6 (5)	C12—N5—C16—C17	−174.8 (3)
C10—N3—C6—N2	179.8 (3)	N6—C16—C17—C18	−1.5 (5)
C10—N3—C6—C7	1.5 (5)	N5—C16—C17—C18	−179.0 (3)
C2—N2—C6—N3	1.4 (6)	C16—C17—C18—C19	−0.9 (6)
C2—N2—C6—C7	179.8 (3)	C17—C18—C19—C20	1.8 (7)
N3—C6—C7—C8	−0.1 (6)	C16—N6—C20—C19	−1.9 (6)
N2—C6—C7—C8	−178.4 (3)	C18—C19—C20—N6	−0.4 (7)

Symmetry code: (i) $-x+1, y, -z+3/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5*B*···O5	0.86	2.07	2.928 (5)	174

N2—H2···N6^{ii}	0.86	2.27	3.129 (4)	176

Symmetry code: (ii) $x, y-1, z$.