IUCrData

ISSN 2414-3146

Dichlorido(pyridine-κN)[2,3,5,6-tetrakis(pyridin-2-yl)pyrazine-κ^3N^2,N^1,N^6]nickel(II)

Kwang Ha*

Chonnam National University, School of Chemical Engineering, Research Institute of Catalysis, Gwangju, Republic of Korea. *Correspondence e-mail: hakwang@chonnam.ac.kr

Received 21 January 2021
Accepted 26 January 2021

Edited by M. Weil, Vienna University of Technology, Austria

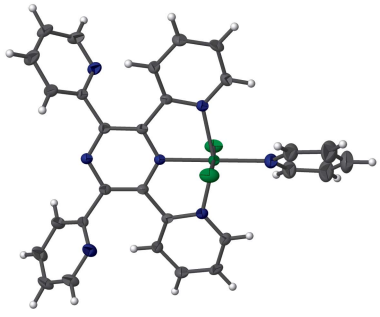
Keywords: crystal structure; nickel(II) complex; pyridine; 2,3,5,6-tetra-2-pyridylpyrazine.

CCDC reference: 2058988

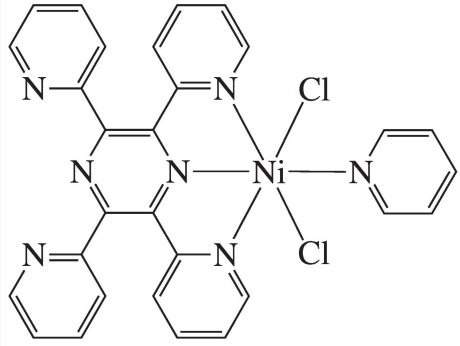
Structural data: full structural data are available from iucrdata.iucr.org

In the title complex, $[NiCl_2(C_5H_5N)(C_{24}H_{16}N_6)]$, the Ni^{II} ion is six-coordinated in a distorted octahedral coordination environment defined by three N atoms of the tridentate 2,3,5,6-tetra-2-pyridylpyrazine ligand, one N atom of the pyridine ligand and two Cl^- anions, with the latter being mutually *trans*. The complex is disposed about a twofold rotation axis along the *a* axis. The complex molecules are connected in the crystal *via* C—H···Cl, C—H···N and π–π [closest inter-centroid separation = 3.7446 (14) Å between pyridyl rings].

3D view



Chemical scheme



Structure description

With reference to the title compound, $[NiCl_2(py)(tppz)]$ (py = pyridine, tppz = 2,3,5,6-tetra-2-pyridylpyrazine), the crystal structures of a related tetranuclear Ni^{II} complex, $[Ni_4Cl_6(tppz)_2(CH_3OH)_4]Cl_2\cdot CH_3OH$ (Winpenny *et al.*, 2005), and of a dinuclear Mn^{II} complex, $[Mn_2Cl_4(tppz)_2]$ (Ha, 2011), have been determined previously.

In the title complex, the central Ni^{II} cation is six-coordinated in a considerably distorted octahedral coordination environment defined by three N atoms of the tridentate tppz ligand, one N atom of the pyridine ligand and two Cl^- anions (Fig. 1). The complex is disposed about a twofold rotation axis along the *a* axis; thus the asymmetric unit contains one half of the complex. The main contribution to the distortion is the tight N—Ni—N chelating angle [<N1—Ni1—N3 = 77.97 (5)°], which results in a non-linear *trans* arrangement of the N3—Ni1—$N3^i$ bonds [<N3—Ni1—$N3^i$ = 155.95 (11)°; symmetry code: (i) $x-y, -y, -z$], whereas the Cl1—Ni1—$Cl1^i$ bonds are almost linear [<Cl1—Ni1—$Cl1^i$ = 175.77 (4)°]. The Ni—*N*[pyrazine(N1) or pyridyl(N3, N5)] bond lengths are roughly equivalent, with distances of 2.008 (3) – 2.1026 (19) Å. The pyrazine ring (N1—$C1^i$) slightly deviates from planarity, with a maximum deviation of 0.057 (2) Å for the C2 atom from the least-squares plane of the ring. The dihedral angles between the nearly planar pyridyl rings and the least-squares plane of their carrier pyrazine ring are

OPEN ACCESS

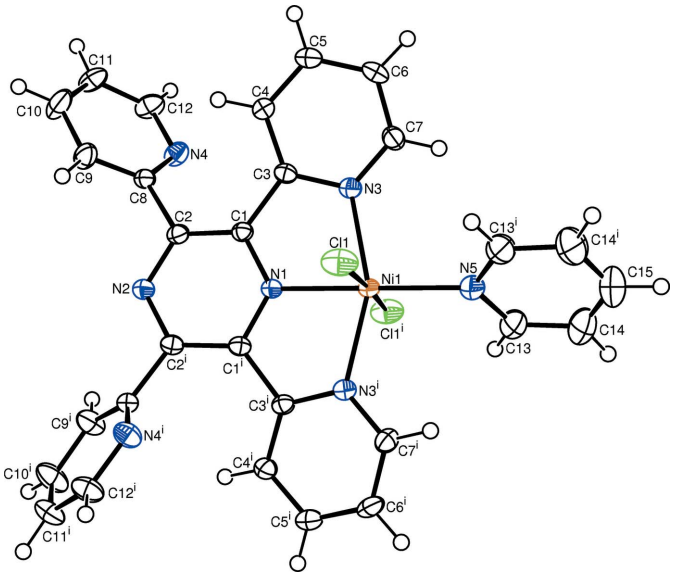


Figure 1
The molecular structure of the title compound showing the atom labelling and displacement ellipsoids drawn at the 50% probability level for all non-H atoms. [Symmetry code: (i) $x-y, -y, -z$.]

14.90 (4)° for the coordinating pyridyl ring (N3—C7) and 54.42 (9)° for the non-coordinating pyridyl ring (N4—C12), respectively. The dihedral angle between the pyrazine ring and the pyridine ligand (N5—C13^{i}) is 57.8 (1)°.

In the crystal, the complex displays numerous inter- and intramolecular π–π interactions between adjacent six-membered rings. The most significant interaction of this kind is that between *Cg*1 (the centroid of the ring N3/C3–C7) and *Cg*1^{ii} [symmetry code: (ii) $x, x-y, -z+\frac{1}{6}$], with a centroid-to-centroid distance of 3.7446 (14) Å and a dihedral angle between the ring planes of 22.24 (12)°. In addition, the complex exhibits inter- and intramolecular C—H···N and C—H···Cl hydrogen bonds (Table 1) that consolidate the three-dimensional packing (Fig. 2).

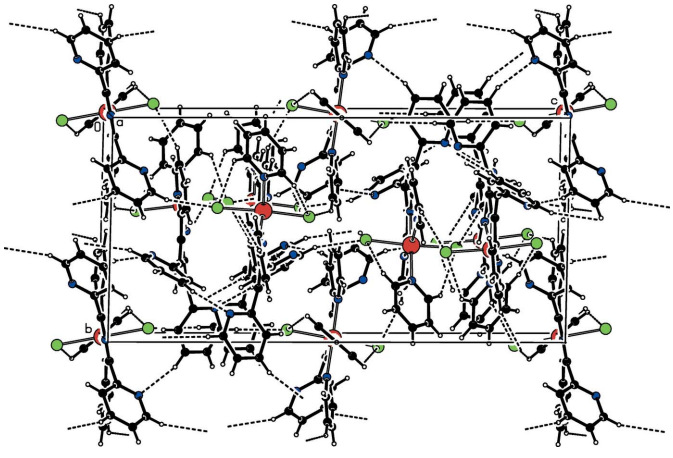


Figure 2
The packing in the crystal of the title compound, viewed approximately along the *a* axis. Hydrogen-bonding interactions are drawn as dashed lines. Colour codes are as in Fig. 1.

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···Cl1^{i}	0.94	2.78	3.513 (3)	136
C10—H10···N4^{ii}	0.94	2.46	3.360 (3)	161
C12—H12···Cl1^{iii}	0.94	2.71	3.602 (3)	160
C13—H13···Cl1^{iv}	0.94	2.68	3.261 (3)	121

Symmetry codes: (i) $x-y, x, z+\frac{1}{6}$; (ii) $y+1, -x+y+1, z-\frac{1}{6}$; (iii) $-y+1, x-y, z+\frac{1}{3}$; (iv) $x-y, -y, -z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[NiCl_2(C_5H_5N)(C_{24}H_{16}N_6)]$
M_r	597.14
Crystal system, space group	Hexagonal, $P6_122$
Temperature (K)	223
a, c (Å)	13.8244 (4), 23.8935 (8)
V (Å^3)	3954.6 (3)
Z	6
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.97
Crystal size (mm)	0.15 × 0.10 × 0.07
Data collection	
Diffractometer	PHOTON 100 CMOS detector
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.700, 0.744
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	125055, 2614, 2412
R_{int}	0.106
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.024, 0.054, 1.08
No. of reflections	2614
No. of parameters	179
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.14
Absolute structure	Flack x determined using 894 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013).
Absolute structure parameter	−0.002 (5)

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *ORTEP-3 for Windows* (Farrugia, 2012).

Synthesis and crystallization

To a solution of $NiCl_2{\cdot}6H_2O$ (0.3779 g, 1.590 mmol) in ethanol (20 ml) was added 2,3,5,6-tetra-2-pyridylpyrazine (0.6220 g, 1.601 mmol), followed by stirring for 24 h at rooom temperature. The formed precipitate was separated by filtration, washed with ethanol and acetone, and dried at 323 K, to give a brown powder (0.5045 g). Brown crystals suitable for X-ray analysis were obtained by slow evaporation from its pyridine/*N*,*N*-dimethylformamide (DMF) solution at 333 K.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The maximum and minimum remaining electron density peaks in the difference Fourier

map are located 0.34 and 0.74 Å, respectively, from atoms C9 and Ni1.

Acknowledgements

The author thanks the KBSI, Seoul Center, for the X-ray data collection.

Funding information

This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (grant No. 2018R1D1A1B07050550).

References

Bruker (2016). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Ha, K. (2011). *Z. Kristallogr. NCS* **226**, 59–60.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Winpenny, R., Lightfoot, K., Parsons, S. & Messenger, D. (2005). *CSD Communication* (refcode: 278243). CCDC, Cambridge, England.

full crystallographic data

IUCrData (2021). **6**, x210094 [https://doi.org/10.1107/S2414314621000948]

Dichlorido(pyridine-κN)[2,3,5,6-tetrakis(pyridin-2-yl)pyrazine-κ^3N^2,N^1,N^6]nickel(II)

Kwang Ha

Dichlorido(pyridine-κN)[2,3,5,6-tetrakis(pyridin-2-yl)pyrazine-κ^3N^2,N^1,N^6]nickel(II)

Crystal data

$[NiCl_2(C_5H_5N)(C_{24}H_{16}N_6)]$
M_r = 597.14
Hexagonal, $P6_122$
a = 13.8244 (4) Å
c = 23.8935 (8) Å
V = 3954.6 (3) Å^3
Z = 6
$F(000)$ = 1836
D_x = 1.504 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9199 reflections
θ = 2.4–26.0°
μ = 0.97 mm^{-1}
T = 223 K
Block, brown
0.15 × 0.10 × 0.07 mm

Data collection

PHOTON 100 CMOS detector diffractometer
Radiation source: sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.700, T_{max} = 0.744
125055 measured reflections
2614 independent reflections
2412 reflections with $I > 2\sigma(I)$
R_{int} = 0.106
θ_{max} = 26.1°, θ_{min} = 2.4°
h = −17→17
k = −17→17
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.054
S = 1.08
2614 reflections
179 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
$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2 + 0.9047P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Absolute structure: Flack x determined using 894 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013).
Absolute structure parameter: −0.002 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.41510 (3)	0.0000	0.0000	0.01866 (12)
Cl1	0.44000 (6)	0.03687 (5)	−0.09968 (3)	0.03369 (17)
N1	0.56034 (18)	0.0000	0.0000	0.0181 (6)
N2	0.75658 (19)	0.0000	0.0000	0.0204 (6)
N3	0.53182 (16)	0.17007 (16)	0.01208 (8)	0.0196 (4)
N4	0.86393 (17)	0.24353 (17)	0.07265 (9)	0.0265 (5)
N5	0.2636 (2)	0.0000	0.0000	0.0303 (7)
C1	0.65538 (19)	0.09724 (18)	0.00453 (10)	0.0177 (5)
C2	0.75545 (19)	0.09505 (19)	0.00914 (9)	0.0194 (5)
C3	0.6391 (2)	0.19584 (19)	0.00471 (10)	0.0187 (5)
C4	0.7236 (2)	0.30472 (19)	−0.00359 (11)	0.0242 (5)
H4	0.7967	0.3205	−0.0114	0.029*
C5	0.6992 (2)	0.3896 (2)	−0.00019 (12)	0.0290 (6)
H5	0.7557	0.4642	−0.0056	0.035*
C6	0.5912 (2)	0.3645 (2)	0.01124 (10)	0.0279 (6)
H6	0.5734	0.4213	0.0157	0.033*
C7	0.5104 (2)	0.2537 (2)	0.01591 (10)	0.0236 (6)
H7	0.4362	0.2361	0.0221	0.028*
C8	0.8647 (2)	0.1935 (2)	0.02484 (10)	0.0199 (5)
C9	0.9581 (2)	0.2297 (2)	−0.00795 (12)	0.0299 (6)
H9	0.9555	0.1912	−0.0408	0.036*
C10	1.0561 (2)	0.3239 (2)	0.00830 (12)	0.0385 (7)
H10	1.1210	0.3514	−0.0137	0.046*
C11	1.0565 (2)	0.3761 (2)	0.05722 (11)	0.0323 (6)
H11	1.1217	0.4403	0.0694	0.039*
C12	0.9594 (2)	0.3327 (2)	0.08824 (11)	0.0309 (6)
H12	0.9608	0.3679	0.1221	0.037*
C13	0.1829 (2)	−0.0605 (2)	0.03686 (14)	0.0414 (7)
H13	0.1959	−0.1024	0.0638	0.050*
C14	0.0811 (3)	−0.0642 (3)	0.03700 (18)	0.0579 (10)
H14	0.0250	−0.1105	0.0624	0.070*
C15	0.0629 (3)	0.0000	0.0000	0.0639 (15)
H15	−0.0051	0.0000	0.0000	0.077*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01813 (17)	0.0145 (2)	0.0222 (2)	0.00723 (11)	0.00093 (9)	0.00185 (17)
Cl1	0.0480 (4)	0.0269 (3)	0.0215 (3)	0.0152 (3)	−0.0012 (3)	0.0025 (2)

N1	0.0175 (10)	0.0147 (13)	0.0210 (14)	0.0073 (7)	−0.0002 (6)	−0.0003 (12)
N2	0.0200 (11)	0.0174 (14)	0.0231 (15)	0.0087 (7)	−0.0006 (6)	−0.0012 (13)
N3	0.0212 (10)	0.0172 (10)	0.0196 (10)	0.0091 (9)	0.0005 (8)	0.0004 (8)
N4	0.0234 (11)	0.0264 (11)	0.0231 (11)	0.0074 (9)	0.0023 (9)	−0.0022 (9)
N5	0.0247 (12)	0.0244 (16)	0.0417 (19)	0.0122 (8)	0.0024 (8)	0.0048 (15)
C1	0.0189 (11)	0.0155 (11)	0.0171 (12)	0.0073 (9)	0.0013 (10)	−0.0007 (9)
C2	0.0195 (12)	0.0165 (12)	0.0194 (12)	0.0069 (10)	0.0017 (10)	0.0010 (10)
C3	0.0220 (12)	0.0163 (11)	0.0176 (11)	0.0095 (10)	−0.0010 (10)	−0.0016 (10)
C4	0.0192 (13)	0.0189 (12)	0.0329 (14)	0.0082 (10)	0.0026 (11)	0.0010 (11)
C5	0.0285 (14)	0.0168 (12)	0.0393 (16)	0.0094 (11)	0.0007 (13)	0.0016 (12)
C6	0.0345 (14)	0.0184 (12)	0.0351 (14)	0.0166 (12)	0.0002 (12)	−0.0012 (11)
C7	0.0257 (13)	0.0237 (13)	0.0254 (14)	0.0153 (11)	0.0025 (10)	0.0015 (10)
C8	0.0186 (12)	0.0160 (12)	0.0241 (13)	0.0080 (10)	−0.0010 (10)	−0.0004 (10)
C9	0.0228 (13)	0.0280 (14)	0.0321 (15)	0.0075 (11)	0.0047 (12)	−0.0085 (12)
C10	0.0206 (14)	0.0381 (16)	0.0406 (18)	0.0025 (12)	0.0078 (12)	−0.0054 (14)
C11	0.0227 (14)	0.0252 (15)	0.0332 (16)	0.0003 (12)	−0.0021 (12)	−0.0018 (12)
C12	0.0319 (14)	0.0260 (14)	0.0232 (13)	0.0057 (12)	−0.0020 (12)	−0.0053 (11)
C13	0.0311 (16)	0.0357 (17)	0.0571 (19)	0.0166 (15)	0.0107 (15)	0.0109 (15)
C14	0.0347 (18)	0.057 (2)	0.082 (3)	0.0222 (17)	0.0195 (18)	0.013 (2)
C15	0.0362 (19)	0.067 (4)	0.098 (5)	0.0336 (18)	0.0005 (18)	0.001 (4)

Geometric parameters (Å, º)

Ni1—N1	2.008 (3)	C4—H4	0.9400
Ni1—N5	2.094 (3)	C5—C6	1.380 (4)
Ni1—N3^{i}	2.1026 (19)	C5—H5	0.9400
Ni1—N3	2.1026 (19)	C6—C7	1.377 (4)
Ni1—Cl1^{i}	2.4238 (6)	C6—H6	0.9400
Ni1—Cl1	2.4238 (6)	C7—H7	0.9400
N1—C1	1.334 (3)	C8—C9	1.373 (3)
N1—C1^{i}	1.334 (3)	C9—C10	1.385 (4)
N2—C2^{i}	1.340 (3)	C9—H9	0.9400
N2—C2	1.340 (3)	C10—C11	1.373 (4)
N3—C7	1.332 (3)	C10—H10	0.9400
N3—C3	1.353 (3)	C11—C12	1.380 (4)
N4—C12	1.332 (3)	C11—H11	0.9400
N4—C8	1.338 (3)	C12—H12	0.9400
N5—C13^{i}	1.337 (3)	C13—C14	1.382 (4)
N5—C13	1.337 (3)	C13—H13	0.9400
C1—C2	1.403 (3)	C14—C15	1.362 (4)
C1—C3	1.488 (3)	C14—H14	0.9400
C2—C8	1.489 (3)	C15—C14^{i}	1.362 (4)
C3—C4	1.382 (3)	C15—H15	0.9400
C4—C5	1.377 (4)		
N1—Ni1—N5	180.0	C5—C4—H4	120.5
N1—Ni1—N3^{i}	77.97 (5)	C3—C4—H4	120.5
N5—Ni1—N3^{i}	102.03 (5)	C4—C5—C6	119.5 (2)

N1—Ni1—N3	77.97 (5)	C4—C5—H5	120.3
N5—Ni1—N3	102.03 (5)	C6—C5—H5	120.3
N3^{i}—Ni1—N3	155.95 (11)	C7—C6—C5	118.0 (2)
N1—Ni1—Cl1^{i}	87.89 (2)	C7—C6—H6	121.0
N5—Ni1—Cl1^{i}	92.11 (2)	C5—C6—H6	121.0
N3^{i}—Ni1—Cl1^{i}	87.19 (5)	N3—C7—C6	123.4 (2)
N3—Ni1—Cl1^{i}	91.94 (5)	N3—C7—H7	118.3
N1—Ni1—Cl1	87.89 (2)	C6—C7—H7	118.3
N5—Ni1—Cl1	92.11 (2)	N4—C8—C9	123.2 (2)
N3^{i}—Ni1—Cl1	91.93 (5)	N4—C8—C2	114.9 (2)
N3—Ni1—Cl1	87.18 (5)	C9—C8—C2	121.9 (2)
Cl1^{i}—Ni1—Cl1	175.77 (4)	C8—C9—C10	118.8 (2)
C1—N1—C1^{i}	122.5 (3)	C8—C9—H9	120.6
C1—N1—Ni1	118.76 (13)	C10—C9—H9	120.6
C1^{i}—N1—Ni1	118.76 (13)	C11—C10—C9	118.6 (2)
C2^{i}—N2—C2	119.7 (3)	C11—C10—H10	120.7
C7—N3—C3	118.1 (2)	C9—C10—H10	120.7
C7—N3—Ni1	126.90 (16)	C10—C11—C12	118.7 (2)
C3—N3—Ni1	113.83 (15)	C10—C11—H11	120.6
C12—N4—C8	117.2 (2)	C12—C11—H11	120.6
C13^{i}—N5—C13	117.1 (4)	N4—C12—C11	123.4 (3)
C13^{i}—N5—Ni1	121.44 (18)	N4—C12—H12	118.3
C13—N5—Ni1	121.44 (18)	C11—C12—H12	118.3
N1—C1—C2	118.0 (2)	N5—C13—C14	122.7 (3)
N1—C1—C3	113.6 (2)	N5—C13—H13	118.7
C2—C1—C3	128.4 (2)	C14—C13—H13	118.7
N2—C2—C1	120.2 (2)	C15—C14—C13	119.4 (4)
N2—C2—C8	115.7 (2)	C15—C14—H14	120.3
C1—C2—C8	124.0 (2)	C13—C14—H14	120.3
N3—C3—C4	121.6 (2)	C14^{i}—C15—C14	118.6 (5)
N3—C3—C1	114.0 (2)	C14^{i}—C15—H15	120.7
C4—C3—C1	124.4 (2)	C14—C15—H15	120.7
C5—C4—C3	119.1 (2)		

C1^{i}—N1—C1—C2	−5.20 (15)	C4—C5—C6—C7	−3.4 (4)
Ni1—N1—C1—C2	174.80 (15)	C3—N3—C7—C6	1.8 (4)
C1^{i}—N1—C1—C3	175.6 (2)	Ni1—N3—C7—C6	−164.88 (19)
Ni1—N1—C1—C3	−4.4 (2)	C5—C6—C7—N3	2.6 (4)
C2^{i}—N2—C2—C1	−5.36 (16)	C12—N4—C8—C9	0.2 (4)
C2^{i}—N2—C2—C8	173.8 (2)	C12—N4—C8—C2	−179.4 (2)
N1—C1—C2—N2	10.7 (3)	N2—C2—C8—N4	−125.1 (2)
C3—C1—C2—N2	−170.2 (2)	C1—C2—C8—N4	54.0 (3)
N1—C1—C2—C8	−168.31 (19)	N2—C2—C8—C9	55.3 (3)
C3—C1—C2—C8	10.8 (4)	C1—C2—C8—C9	−125.6 (3)
C7—N3—C3—C4	−5.6 (4)	N4—C8—C9—C10	−1.4 (4)
Ni1—N3—C3—C4	162.80 (19)	C2—C8—C9—C10	178.1 (3)
C7—N3—C3—C1	176.4 (2)	C8—C9—C10—C11	1.3 (5)
Ni1—N3—C3—C1	−15.3 (3)	C9—C10—C11—C12	0.1 (5)

N1—C1—C3—N3	13.1 (3)	C8—N4—C12—C11	1.3 (4)
C2—C1—C3—N3	−166.0 (2)	C10—C11—C12—N4	−1.4 (5)
N1—C1—C3—C4	−164.9 (2)	C13^{i}—N5—C13—C14	1.5 (3)
C2—C1—C3—C4	16.0 (4)	Ni1—N5—C13—C14	−178.5 (3)
N3—C3—C4—C5	4.8 (4)	N5—C13—C14—C15	−3.1 (5)
C1—C3—C4—C5	−177.3 (2)	C13—C14—C15—C14^{i}	1.5 (3)
C3—C4—C5—C6	−0.2 (4)		

Symmetry code: (i) *x*−*y*, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···Cl1^{ii}	0.94	2.78	3.513 (3)	136
C10—H10···N4^{iii}	0.94	2.46	3.360 (3)	161
C12—H12···Cl1^{iv}	0.94	2.71	3.602 (3)	160
C13—H13···Cl1^{i}	0.94	2.68	3.261 (3)	121

Symmetry codes: (i) *x*−*y*, −*y*, −*z*; (ii) *x*−*y*, *x*, *z*+1/6; (iii) *y*+1, −*x*+*y*+1, *z*−1/6; (iv) −*y*+1, *x*−*y*, *z*+1/3.