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Di-μ_2-chlorido-bis{chlorido[2,4,6-tris(pyridin-2-yl)-1,3,5-triazine-κ^3N^2,N^1,N^6]nickel(II)}

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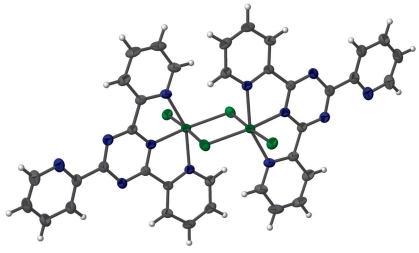
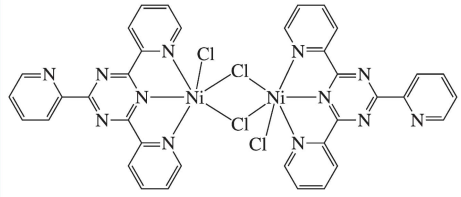
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[Ni_2Cl_4(C_{18}H_{12}N_6)_2]$, the Ni^{II} ions are hexa-coordinated in a distorted octahedral coordination environment defined by three N atoms of the tridentate 2,4,6-tri-2-pyridyl-1,3,5-triazine ligand and three Cl^- anions in a meridional geometry. The two Ni^{II} ions are bridged by two Cl anionic ligands, thereby forming a dinuclear complex. A crystallographic centre of inversion is located at the centroid of the Ni_2Cl_2 ring.

3D view



Chemical scheme



Structure description

With reference to the title compound, $[Ni_2Cl_4(tptz)_2]$ (tptz = 2,4,6-tri-2-pyridyl-1,3,5-triazine), the crystal structures of related chlorido Ni^{II} complexes $[NiCl_2(tptz)(CH_3OH)]$ (Hadadzadeh *et al.*, 2012), $[NiCl(H\text{-}tptz)(H_2O)_2]Cl_2{\cdot}2H_2O$ (Zibaseresht & Hartshorn, 2005) and $[NiCl_2(py)(tptz)]$ (py = pyridine) (Ha, 2019) have been determined previously.

In the complex, the two Ni^{II} cations are bridged by two chlorido ligands to form a dinuclear complex. A crystallographic centre of inversion is located at the centroid of the Ni_2Cl_2 ring. The asymmetric unit therefore contains one half of the complex (Fig. 1). Each Ni^{II} atom is hexa-coordinated in a considerably distorted octahedral coordination environment defined by three N atoms of the tridentate tptz ligand, two bridging Cl^- ligands and one terminal Cl^- anion. The main contributions to the distortion are the tight N—Ni—N chelating angles [N1—Ni1—N4 = 76.96 (6)° and N1—Ni1—N6 = 77.52 (6)°] and the chlorido bridges, which result in a non-linear *trans* arrangement of the N4—Ni1—N6 and N1—Ni1—Cl axes [N4—Ni1—N6 = 154.46 (6)° and N1—Ni1—Cl1 = 169.87 (5)°]. On the other hand the Cl2—Ni1—$Cl1^i$ axis (symmetry code: (i) $-x, -y+1, -z$) is almost linear [Cl2—Ni1—$Cl1^i$ = 176.25 (2)°]. The Ni—N(pyridyl) bonds [Ni1—N4/N6 = 2.130 (2) and 2.129 (2) Å] are slightly longer than the Ni—N(triazine) bond [Ni1—N1 = 1.970 (2) Å]. The three Ni—Cl bond lengths are somewhat different [Ni1—$Cl1^i$ = 2.5812 (5), Ni1—Cl1 = 2.3326 (5) and Ni1—Cl2 = 2.3538 (5) Å]. The two pyridyl rings

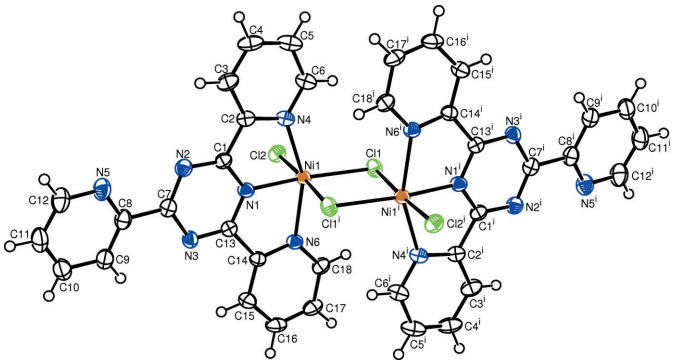


Figure 1
Molecular structure of the title compound showing the atom labelling and displacement ellipsoids drawn at the 50% probability level for non-H atoms. Symmetry code: (i) $-x, -y+1, -z$.

that coordinat to the Ni^{II} atom are located approximately parallel to the respective triazine ring, making dihedral angles of 4.51 (6) and 4.95 (6)°, respectively. The dihedral angle between the non-coordinating pyridyl substituent and the triazine ring is 7.56 (6)°.

The complex displays numerous intermolecular π–π interactions between adjacent six-membered rings. For *Cg*1 (the centroid of ring N5/C8–C12) and *Cg*2^{ii} [the centroid of ring N6/C14–C18; symmetry code: (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$], the centroid–centroid distance is 4.138 (1) Å and the dihedral angle between the ring planes is 5.44 (10)°. In addition, the complex reveals intermolecular C—H···Cl hydrogen bonds with distances of 2.773 (3)–3.605 (2) Å between the donor and acceptor atoms, to stabilize the crystal structure (Table 1, Fig. 2).

Synthesis and crystallization

To a solution of $NiCl_2{\cdot}6\,H_2O$ (0.2670 g, 1.123 mmol) in ethanol (30 ml) was added 2,4,6-tri-2-pyridyl-1,3,5-triazine (0.2814 g, 0.901 mmol). The solution was stirred for 12 h at room temperature. The formed precipitate was separated by filtration, washed with ethanol and acetone, and dried at 323 K, to give a pale-green powder (0.3363 g, 84%). Brown crystals suitable for X-ray analysis were obtained by slow evaporation from a dimethyl sulfoxide (DMSO) solution at 363 K.

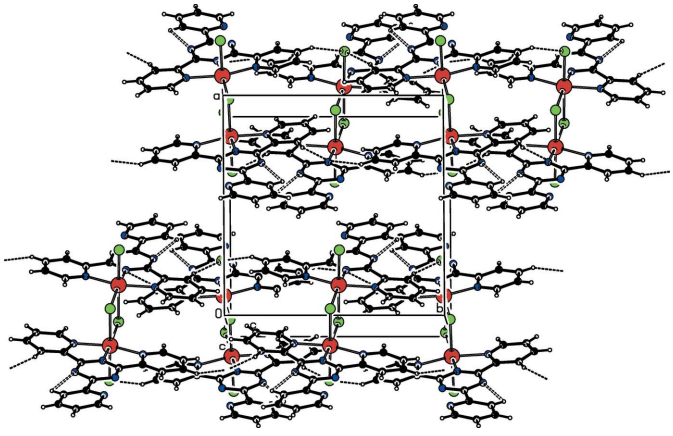


Figure 2
Crystal structure of the title compound showing π–π interactions as well as weak C–H···Cl hydrogen bonds.

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···Cl2^{i}	0.94	2.76	3.605 (2)	150
C15—H15···Cl2^{ii}	0.94	2.57	3.471 (2)	162

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Ni_2Cl_4(C_{18}H_{12}N_6)_2]$
M_r	883.89
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	223
a, b, c (Å)	13.0130 (4), 12.8275 (4), 11.0153 (3)
β (°)	106.5083 (11)
V (Å^3)	1762.93 (9)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.42
Crystal size (mm)	0.25 × 0.15 × 0.13
Data collection	
Diffractometer	PHOTON 100 CMOS detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.660, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	48040, 3487, 2828
R_{int}	0.059
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.028, 0.067, 1.06
No. of reflections	3487
No. of parameters	244
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.20

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT2014/7* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The remaining maximum (0.33 e Å^{-3}) and minimum (−0.20 e Å^{-3}) electron density in the difference Fourier map are located 0.73 and 1.28 Å, respectively, from atoms C2 and C9.

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References

Bruker (2016). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Ha, K. (2019). *Z. Kristallogr. NCS* **234**, 775–776.
Hadadzadeh, H., Maghami, M., Simpson, J., Khalaji, A. D. & Abdi, K. (2012). *J. Chem. Crystallogr.* **42**, 656–667.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.
Zibaseresht, R. & Hartshorn, R. M. (2005). *Aust. J. Chem.* **58**, 345–353.

full crystallographic data

IUCrData (2021). **6**, x210093 [https://doi.org/10.1107/S2414314621000936]

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Crystal data

$[Ni_2Cl_4(C_{18}H_{12}N_6)_2]$
M_r = 883.89
Monoclinic, $P2_1/c$
a = 13.0130 (4) Å
b = 12.8275 (4) Å
c = 11.0153 (3) Å
β = 106.5083 (11)°
V = 1762.93 (9) Å^3
Z = 2
$F(000)$ = 896
D_x = 1.665 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9969 reflections
θ = 2.3–28.2°
μ = 1.42 mm^{-1}
T = 223 K
Block, brown
0.25 × 0.15 × 0.13 mm

Data collection

PHOTON 100 CMOS detector diffractometer
Radiation source: sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.660, T_{max} = 0.745
48040 measured reflections
3487 independent reflections
2828 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 26.1°, θ_{min} = 2.3°
h = −16→16
k = −15→15
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.067
S = 1.06
3487 reflections
244 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
$w = 1/[\sigma^2(F_o^2) + (0.0314P)^2 + 0.698P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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.

Refinement. Hydrogen atoms on C atoms were positioned geometrically and allowed to ride on their respective parent atoms: C—H = 0.94 Å and U_{iso}(H) = 1.2 U_{eq}(C).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.14246 (2)	0.51866 (2)	0.04761 (2)	0.02427 (9)
Cl1	0.01562 (4)	0.48538 (4)	−0.14563 (4)	0.02986 (13)
Cl2	0.29409 (4)	0.52462 (4)	−0.02845 (5)	0.03079 (13)
N1	0.22767 (13)	0.54763 (12)	0.22294 (15)	0.0248 (4)
N2	0.32398 (14)	0.48592 (13)	0.42305 (15)	0.0287 (4)
N3	0.29552 (13)	0.66875 (13)	0.38378 (15)	0.0276 (4)
N4	0.18958 (13)	0.36721 (12)	0.12204 (15)	0.0267 (4)
N5	0.42794 (15)	0.52970 (14)	0.66906 (16)	0.0374 (4)
N6	0.13351 (12)	0.68398 (12)	0.05789 (14)	0.0247 (4)
C1	0.26891 (15)	0.47112 (15)	0.30292 (18)	0.0246 (4)
C2	0.24779 (16)	0.36589 (15)	0.24522 (18)	0.0256 (4)
C3	0.28603 (17)	0.27542 (16)	0.3092 (2)	0.0339 (5)
H3	0.3234	0.2769	0.3958	0.041*
C4	0.26843 (19)	0.18244 (17)	0.2435 (2)	0.0409 (6)
H4	0.2930	0.1192	0.2848	0.049*
C5	0.21447 (19)	0.18388 (17)	0.1169 (2)	0.0413 (6)
H5	0.2045	0.1219	0.0696	0.050*
C6	0.17494 (17)	0.27710 (15)	0.0595 (2)	0.0324 (5)
H6	0.1364	0.2769	−0.0268	0.039*
C7	0.33706 (15)	0.58634 (16)	0.45819 (18)	0.0278 (4)
C8	0.39884 (16)	0.61154 (17)	0.59008 (19)	0.0302 (5)
C9	0.42105 (16)	0.71422 (18)	0.6268 (2)	0.0338 (5)
H9	0.3990	0.7689	0.5684	0.041*
C10	0.47666 (17)	0.73425 (19)	0.7519 (2)	0.0394 (6)
H10	0.4937	0.8030	0.7802	0.047*
C11	0.50621 (18)	0.6520 (2)	0.8335 (2)	0.0426 (6)
H11	0.5435	0.6635	0.9190	0.051*
C12	0.48059 (18)	0.5520 (2)	0.7888 (2)	0.0438 (6)
H12	0.5015	0.4964	0.8462	0.053*
C13	0.23995 (15)	0.64467 (15)	0.26684 (18)	0.0237 (4)
C14	0.18376 (15)	0.72372 (15)	0.17355 (18)	0.0238 (4)
C15	0.18125 (16)	0.82788 (15)	0.2024 (2)	0.0301 (5)
H15	0.2164	0.8528	0.2839	0.036*
C16	0.12571 (17)	0.89494 (16)	0.1083 (2)	0.0350 (5)
H16	0.1212	0.9663	0.1255	0.042*
C17	0.07695 (17)	0.85609 (16)	−0.0108 (2)	0.0336 (5)
H17	0.0406	0.9009	−0.0766	0.040*
C18	0.08231 (15)	0.75012 (16)	−0.03215 (19)	0.0287 (5)
H18	0.0485	0.7239	−0.1134	0.034*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.03109 (15)	0.01883 (14)	0.02120 (14)	0.00130 (10)	0.00470 (11)	0.00041 (10)
Cl1	0.0330 (3)	0.0344 (3)	0.0216 (2)	−0.0031 (2)	0.0068 (2)	−0.0029 (2)
Cl2	0.0314 (3)	0.0313 (3)	0.0298 (3)	0.0037 (2)	0.0088 (2)	0.0046 (2)
N1	0.0300 (9)	0.0208 (8)	0.0235 (8)	0.0015 (7)	0.0073 (7)	0.0012 (7)
N2	0.0311 (9)	0.0288 (9)	0.0254 (9)	0.0020 (7)	0.0066 (7)	0.0031 (7)
N3	0.0288 (9)	0.0281 (9)	0.0239 (9)	−0.0008 (7)	0.0044 (7)	−0.0001 (7)
N4	0.0331 (9)	0.0217 (9)	0.0280 (9)	−0.0003 (7)	0.0130 (7)	−0.0009 (7)
N5	0.0392 (11)	0.0432 (11)	0.0257 (9)	−0.0010 (9)	0.0028 (8)	0.0043 (8)
N6	0.0283 (9)	0.0215 (9)	0.0246 (9)	0.0013 (7)	0.0079 (7)	0.0015 (7)
C1	0.0256 (10)	0.0243 (10)	0.0249 (10)	0.0028 (8)	0.0088 (8)	0.0034 (8)
C2	0.0301 (11)	0.0237 (10)	0.0260 (10)	0.0024 (8)	0.0129 (8)	0.0027 (8)
C3	0.0400 (12)	0.0304 (12)	0.0350 (12)	0.0078 (9)	0.0165 (10)	0.0107 (10)
C4	0.0541 (15)	0.0222 (11)	0.0527 (15)	0.0098 (10)	0.0253 (12)	0.0115 (10)
C5	0.0569 (15)	0.0214 (11)	0.0533 (15)	−0.0005 (10)	0.0280 (12)	−0.0030 (10)
C6	0.0440 (13)	0.0241 (11)	0.0332 (12)	−0.0018 (9)	0.0177 (10)	−0.0026 (9)
C7	0.0258 (11)	0.0324 (11)	0.0257 (10)	0.0007 (9)	0.0081 (8)	0.0014 (9)
C8	0.0259 (11)	0.0396 (13)	0.0252 (10)	0.0003 (9)	0.0073 (9)	0.0018 (9)
C9	0.0294 (11)	0.0392 (13)	0.0307 (11)	0.0010 (9)	0.0051 (9)	0.0000 (10)
C10	0.0309 (12)	0.0491 (15)	0.0368 (13)	−0.0024 (11)	0.0075 (10)	−0.0112 (11)
C11	0.0362 (13)	0.0603 (16)	0.0269 (12)	−0.0022 (12)	0.0019 (10)	−0.0053 (11)
C12	0.0429 (14)	0.0539 (15)	0.0289 (12)	−0.0010 (12)	0.0012 (10)	0.0068 (11)
C13	0.0239 (10)	0.0241 (10)	0.0242 (10)	0.0001 (8)	0.0083 (8)	0.0012 (8)
C14	0.0252 (10)	0.0213 (10)	0.0262 (10)	−0.0006 (8)	0.0092 (8)	−0.0001 (8)
C15	0.0347 (12)	0.0236 (11)	0.0322 (11)	−0.0021 (9)	0.0095 (9)	−0.0030 (9)
C16	0.0401 (13)	0.0187 (11)	0.0492 (14)	0.0022 (9)	0.0174 (11)	0.0017 (10)
C17	0.0349 (12)	0.0252 (11)	0.0414 (13)	0.0069 (9)	0.0119 (10)	0.0106 (10)
C18	0.0298 (11)	0.0291 (11)	0.0277 (11)	0.0039 (9)	0.0090 (9)	0.0058 (8)

Geometric parameters (Å, º)

Ni1—N1	1.9700 (16)	C4—C5	1.372 (3)
Ni1—N6	2.1286 (16)	C4—H4	0.9400
Ni1—N4	2.1300 (16)	C5—C6	1.382 (3)
Ni1—Cl1	2.3326 (5)	C5—H5	0.9400
Ni1—Cl2	2.3538 (5)	C6—H6	0.9400
Ni1—Cl1^{i}	2.5812 (5)	C7—C8	1.482 (3)
Cl1—Ni1^{i}	2.5811 (5)	C8—C9	1.384 (3)
N1—C1	1.326 (2)	C9—C10	1.387 (3)
N1—C13	1.329 (2)	C9—H9	0.9400
N2—C1	1.327 (3)	C10—C11	1.368 (3)
N2—C7	1.342 (3)	C10—H10	0.9400
N3—C13	1.322 (2)	C11—C12	1.381 (3)
N3—C7	1.353 (3)	C11—H11	0.9400
N4—C6	1.331 (3)	C12—H12	0.9400
N4—C2	1.353 (2)	C13—C14	1.481 (3)

N5—C12	1.333 (3)	C14—C15	1.376 (3)
N5—C8	1.347 (3)	C15—C16	1.382 (3)
N6—C18	1.331 (2)	C15—H15	0.9400
N6—C14	1.355 (2)	C16—C17	1.379 (3)
C1—C2	1.484 (3)	C16—H16	0.9400
C2—C3	1.375 (3)	C17—C18	1.385 (3)
C3—C4	1.380 (3)	C17—H17	0.9400
C3—H3	0.9400	C18—H18	0.9400

N1—Ni1—N6	77.52 (6)	C4—C5—H5	120.2
N1—Ni1—N4	76.96 (6)	C6—C5—H5	120.2
N6—Ni1—N4	154.46 (6)	N4—C6—C5	122.3 (2)
N1—Ni1—Cl1	169.87 (5)	N4—C6—H6	118.8
N6—Ni1—Cl1	101.28 (4)	C5—C6—H6	118.8
N4—Ni1—Cl1	103.65 (5)	N2—C7—N3	125.40 (18)
N1—Ni1—Cl2	92.73 (5)	N2—C7—C8	118.76 (18)
N6—Ni1—Cl2	92.90 (4)	N3—C7—C8	115.81 (18)
N4—Ni1—Cl2	89.31 (5)	N5—C8—C9	123.76 (19)
Cl1—Ni1—Cl2	97.384 (19)	N5—C8—C7	115.95 (18)
N1—Ni1—Cl1^{i}	83.52 (5)	C9—C8—C7	120.27 (19)
N6—Ni1—Cl1^{i}	86.30 (4)	C8—C9—C10	118.3 (2)
N4—Ni1—Cl1^{i}	89.84 (5)	C8—C9—H9	120.9
Cl1—Ni1—Cl1^{i}	86.370 (18)	C10—C9—H9	120.9
Cl2—Ni1—Cl1^{i}	176.246 (19)	C11—C10—C9	118.7 (2)
Ni1—Cl1—Ni1^{i}	93.631 (18)	C11—C10—H10	120.7
C1—N1—C13	117.87 (17)	C9—C10—H10	120.7
C1—N1—Ni1	121.36 (13)	C10—C11—C12	119.2 (2)
C13—N1—Ni1	120.64 (13)	C10—C11—H11	120.4
C1—N2—C7	114.41 (17)	C12—C11—H11	120.4
C13—N3—C7	114.93 (17)	N5—C12—C11	123.8 (2)
C6—N4—C2	117.72 (17)	N5—C12—H12	118.1
C6—N4—Ni1	127.55 (14)	C11—C12—H12	118.1
C2—N4—Ni1	114.53 (12)	N3—C13—N1	123.33 (18)
C12—N5—C8	116.3 (2)	N3—C13—C14	122.80 (17)
C18—N6—C14	117.79 (17)	N1—C13—C14	113.86 (16)
C18—N6—Ni1	128.22 (13)	N6—C14—C15	123.07 (18)
C14—N6—Ni1	113.93 (12)	N6—C14—C13	113.96 (16)
N1—C1—N2	123.94 (18)	C15—C14—C13	122.96 (18)
N1—C1—C2	113.45 (17)	C14—C15—C16	118.22 (19)
N2—C1—C2	122.61 (17)	C14—C15—H15	120.9
N4—C2—C3	122.83 (19)	C16—C15—H15	120.9
N4—C2—C1	113.64 (16)	C17—C16—C15	119.33 (19)
C3—C2—C1	123.51 (18)	C17—C16—H16	120.3
C2—C3—C4	118.6 (2)	C15—C16—H16	120.3
C2—C3—H3	120.7	C16—C17—C18	119.0 (2)
C4—C3—H3	120.7	C16—C17—H17	120.5
C5—C4—C3	118.8 (2)	C18—C17—H17	120.5
C5—C4—H4	120.6	N6—C18—C17	122.54 (19)

C3—C4—H4	120.6	N6—C18—H18	118.7
C4—C5—C6	119.6 (2)	C17—C18—H18	118.7
C13—N1—C1—N2	−1.8 (3)	N2—C7—C8—C9	174.92 (19)
Ni1—N1—C1—N2	−177.77 (14)	N3—C7—C8—C9	−6.9 (3)
C13—N1—C1—C2	178.24 (16)	N5—C8—C9—C10	0.2 (3)
Ni1—N1—C1—C2	2.3 (2)	C7—C8—C9—C10	178.34 (18)
C7—N2—C1—N1	−1.2 (3)	C8—C9—C10—C11	−0.6 (3)
C7—N2—C1—C2	178.72 (17)	C9—C10—C11—C12	0.5 (3)
C6—N4—C2—C3	−4.1 (3)	C8—N5—C12—C11	−0.4 (3)
Ni1—N4—C2—C3	−179.45 (15)	C10—C11—C12—N5	0.0 (4)
C6—N4—C2—C1	174.13 (17)	C7—N3—C13—N1	−1.9 (3)
Ni1—N4—C2—C1	−1.2 (2)	C7—N3—C13—C14	176.77 (17)
N1—C1—C2—N4	−0.6 (2)	C1—N1—C13—N3	3.5 (3)
N2—C1—C2—N4	179.51 (17)	Ni1—N1—C13—N3	179.50 (14)
N1—C1—C2—C3	177.70 (18)	C1—N1—C13—C14	−175.29 (16)
N2—C1—C2—C3	−2.2 (3)	Ni1—N1—C13—C14	0.7 (2)
N4—C2—C3—C4	3.0 (3)	C18—N6—C14—C15	2.1 (3)
C1—C2—C3—C4	−175.10 (19)	Ni1—N6—C14—C15	−175.50 (15)
C2—C3—C4—C5	0.6 (3)	C18—N6—C14—C13	−179.03 (16)
C3—C4—C5—C6	−2.9 (3)	Ni1—N6—C14—C13	3.4 (2)
C2—N4—C6—C5	1.7 (3)	N3—C13—C14—N6	178.41 (17)
Ni1—N4—C6—C5	176.33 (16)	N1—C13—C14—N6	−2.8 (2)
C4—C5—C6—N4	1.8 (3)	N3—C13—C14—C15	−2.7 (3)
C1—N2—C7—N3	3.0 (3)	N1—C13—C14—C15	176.14 (18)
C1—N2—C7—C8	−179.11 (17)	N6—C14—C15—C16	−0.7 (3)
C13—N3—C7—N2	−1.5 (3)	C13—C14—C15—C16	−179.52 (18)
C13—N3—C7—C8	−179.46 (17)	C14—C15—C16—C17	−1.3 (3)
C12—N5—C8—C9	0.3 (3)	C15—C16—C17—C18	1.8 (3)
C12—N5—C8—C7	−177.95 (19)	C14—N6—C18—C17	−1.4 (3)
N2—C7—C8—N5	−6.8 (3)	Ni1—N6—C18—C17	175.71 (15)
N3—C7—C8—N5	171.38 (17)	C16—C17—C18—N6	−0.5 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···Cl2^{ii}	0.94	2.76	3.605 (2)	150
C15—H15···Cl2^{iii}	0.94	2.57	3.471 (2)	162

Symmetry codes: (ii) $x, -y+1/2, z+1/2$; (iii) $x, -y+3/2, z+1/2$.