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Tris(propane-1,2-diamine-κ^2N,N')-nickel(II) tetracyanidonickelate(II)

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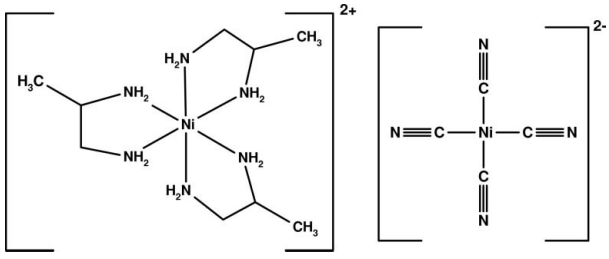
Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.037; wR factor = 0.101; data-to-parameter ratio = 10.6.

The title compound, $[Ni(C_3H_{10}N_2)_3][Ni(CN)_4]$, is built up of $[Ni(pn)_3]^{2+}$ cations (pn is 1,2-diaminopropane) and $[Ni(CN)_4]^{2-}$ anions. Both Ni^{II} atoms in the cation and the anion lie on a mirror plane. The respective ions interact through Coulombic forces and through a complex network of hydrogen bonds. Extended disorder associated with the cation has been resolved. The occupancies of the respective disordered positions are 0.4:0.4:0.2.

Related literature

For related literature, see: Paharová *et al.* (2007); Rodriguez *et al.* (1999); Saha *et al.* (2005); Smékal *et al.* (2001); Černák *et al.* (2002); Bubanec *et al.* (2004); Potočňák *et al.* (2008).



Experimental

Crystal data

$[Ni(C_3H_{10}N_2)_3][Ni(CN)_4]$
M_r = 443.89
Orthorhombic, *Pnma*
a = 9.7310 (12) Å
b = 13.3770 (14) Å
c = 16.275 (3) Å
V = 2118.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.79 mm^{-1}
T = 193 (2) K
0.5 × 0.1 × 0.1 mm

Data collection

Stoe IPDS diffractometer
Absorption correction: Gaussian (*XPREP* in *SHELXTL*; Siemens, 1996)
T_{min} = 0.580, T_{max} = 0.815
14468 measured reflections
1947 independent reflections
1401 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 0.92
1947 reflections
183 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—C1	1.852 (7)	Ni2—N9	2.128 (6)
Ni1—C2	1.856 (4)	Ni2—N5	2.135 (6)
Ni1—C3	1.866 (7)	Ni2—N4	2.137 (6)
Ni2—N7	2.112 (6)	Ni2—N6	2.139 (5)
Ni2—N8	2.122 (6)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···N2^{i}	0.92	2.24	3.140 (7)	167
N5—H5A···N2^{ii}	0.92	2.17	3.083 (6)	169
N5—H5B···N3	0.92	2.30	3.180 (8)	159
N6—H6A···N2^{i}	0.92	2.23	3.073 (7)	152
N6—H6B···N3	0.92	2.54	3.349 (7)	147
N7—H7A···N1^{iii}	0.92	2.42	3.295 (8)	158
N7—H7B···N1^{iv}	0.92	2.36	3.159 (7)	145
N8—H8A···N1^{iii}	0.92	2.07	2.985 (8)	179
N9—H9A···N2^{ii}	0.92	2.42	3.212 (8)	144

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

Data collection: *EXPOSE* in *IPDS* (Stoe & Cie, 1999); cell refinement: *CELL* in *IPDS*; data reduction: *INTEGRATE* in *IPDS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *PARST* (Nardelli, 1983) and *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2004); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2155).

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supporting information

Acta Cryst. (2008). E**64**, m324–m325 [doi:10.1107/S1600536807068420]

Tris(propane-1,2-diamine-κ^2N,N')nickel(II) tetracyanidonickelate(II)

Juraj Kuchár and Juraj Černák

S1. Comment

The title compound, $C_{13}H_{30}N_{10}Ni_2$, was studied as part of a broader study of cyanocomplexes viewed as magnetic materials [Černák *et al.*2002). The complex is ionic and built up of $[Ni(pn)_3]^{2+}$cations (pn: 1,2-diaminopropane) and $[Ni(CN)\sim4\sim]^{2-}$ anions. Other similar ionic compounds with square tetracyanometallates(II) and $[M(L—L)_3]^{2+}$ cations (*M* = Ni, Zn, Cd; L—*L*: a chelating ligand), have already been described [Bubanec *et al.*, 2004; Rodriguez *et al.*, 1999; Paharová *et al.*, 2007]. The Pt analogue was described by Potočňák *et al.* (2008).

The Ni^{II} atom in the complex cation exhibits pseudo-octahedral coordination by six nitrogen atoms from three chelate bonded *pn* ligands in *gauche* conformations. As the nickel atom occupies the position on a mirror plane the chelate bonded ligands are disordered in two positions with half occupancy (Fig. 1). Further disorder associated with the position of the methyl groups bonded to the carbon atom was detected so within the same metallocycle both *R* and *S* enantiomers are present with the same occupancy. Moreover, the structure is centrosymmetric so both opposite absolute configurations $\Lambda\delta\delta\lambda$ and $\Delta\lambda\lambda\delta$ of the chiral cations are present in the unit cell in equal quantities. It is worth noting that for the synthesis a racemic mixture of the *pn* ligand was used. The observed geometrical parameters are close to those observed in $[Ni(pn)_3][Fe(CN)_5NO].H_2O$ [Saha *et al.*, 2005].

The charge of the cation is compensated by a $[Ni(CN)_4]^{2-}$ anion. The latter is bisected by a mirror plane, leading to a rather regular NiC_4 chromophore. The geometric characteristics are similar to those previously reported [Smékal *et al.*, 2001].

The Ni^{II} atoms in the respective ions are not connected by covalent bonds, the shortest distance between Ni^{II} atoms being 8.527 (1) Å. The cations are connected by a complicated system of weak intermolecular hydrogen bonds of the N—H···N≡C—Ni—C≡N···H—N type, in which also the complex anions take part and where the H···N distance range is 2.103–2.488 Å.

S2. Experimental

To 10 ml of a 0.1 *M* hot solution of $NiSO_4.6H_2O$ (0.262 g, 1 mmol) 0.35 ml of pn (4 mmol) were added under continuous stirring, followed by addition of 10 ml of a 0.1 *M* warm solution of $K_2[Ni(CN)_4].H_2O$ (1 mmol). The resulting clear solution was left for crystallization at room temperature. Single crystals of the title compound, in the form of light violet needles suitable for X-ray studies, appeared after one day.

S3. Refinement

The structure was solved by direct method. The model (including two 50:50% disordered positions of the pn ligands, forced by the crystallographic mirror symmetry in the cation) was completed by subsequent Fourier syntheses. At this stage the calculated difference Fourier map indicated the presence of further positional disorder of the methyl groups in the pn ligands. The occupational factors refined by fixing the common isotropic thermal parameters of the concerning

carbon atoms indicated 50:50 occupancy which was in the subsequent refinement cycles fixed. Finally, the hydrogen atoms were put in the calculated positions taking into account the observed disorder. Anisotropic thermal parameters were refined for all non-H atoms. All H atoms positions were calculated using the appropriate riding model with isotropic temperature factors being 1.2 times larger then temperature factors of their parent atoms. Geometrical analysis was performed using *PARST* (Nardelli, 1983) and *SHELXL97*.

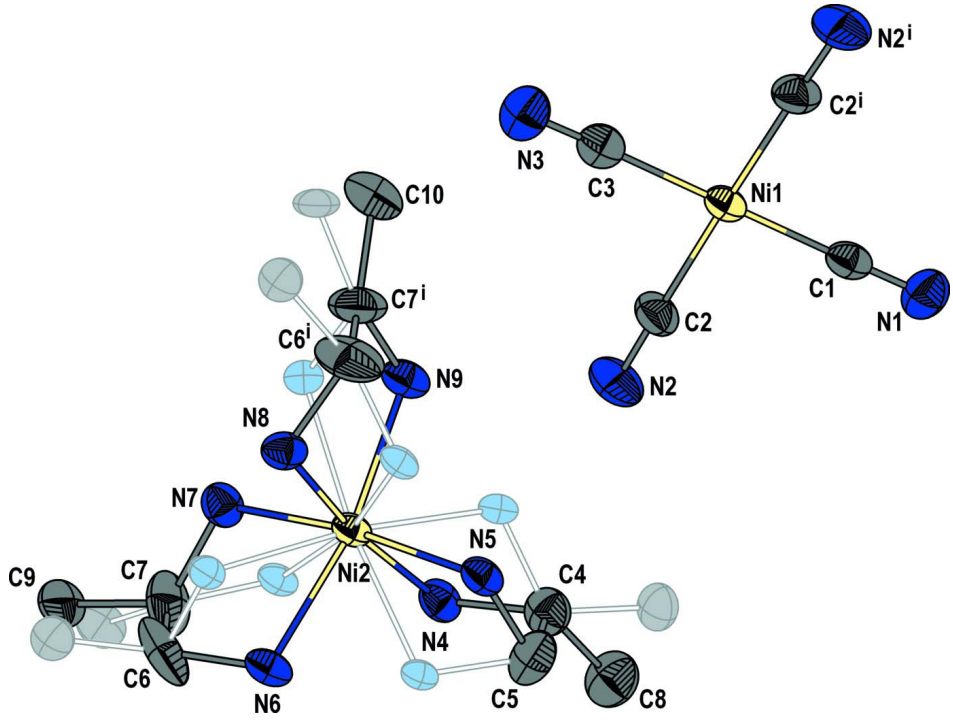

Figure 1

View of the complex cation and complex anion of the title compound. The thermal ellipsoids are drawn at 30% probability level. The disordered positions in the complex cation are shown with light colors (i: *x*, 0.5 - *y*, *z*).

Tris(propane-1,2-diamine-κ^2N,N')nickel(II) tetracyanidonickelate(II)

Crystal data

$[Ni(C_3H_{10}N_2)_3][Ni(CN)_4]$
M_r = 443.89
Orthorhombic, *Pnma*
Hall symbol: -P 2ac 2n
a = 9.7310 (12) Å
b = 13.3770 (14) Å
c = 16.275 (3) Å
V = 2118.5 (5) Å^3
Z = 4
F(000) = 936
D_x = 1.392 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 1308 reflections
θ = 4.6–30.5°
μ = 1.79 mm^{-1}
T = 193 K
Needle, light-violet
0.5 × 0.1 × 0.1 mm

Data collection

Stoe IPDS diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 150 pixels mm^{-1}
φ scans
Absorption correction: gaussian (*XPREP* in *SHELXTL*; Siemens, 1996)
T_{min} = 0.580, T_{max} = 0.815
14468 measured reflections
1947 independent reflections
1401 reflections with $I > 2\sigma(I)$

R_{int} = 0.052
θ_{max} = 25.0°, θ_{min} = 2.9°
h = −11→11
k = −15→15
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 0.92
1947 reflections
183 parameters
12 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
$w = 1/[\sigma^2(F_o^2) + (0.0714P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Ni1	0.79310 (7)	0.2500	0.07496 (4)	0.0430 (2)	
C1	0.8878 (6)	0.2500	0.1736 (4)	0.0505 (13)	
N1	0.9497 (6)	0.2500	0.2336 (3)	0.0711 (14)	
C2	0.7945 (5)	0.1112 (3)	0.0757 (3)	0.0605 (10)	
N2	0.7977 (6)	0.0261 (3)	0.0772 (3)	0.0972 (15)	
C3	0.6984 (5)	0.2500	−0.0248 (4)	0.0554 (14)	
N3	0.6348 (6)	0.2500	−0.0840 (4)	0.0746 (15)	
Ni2	0.26627 (6)	0.2500	0.03265 (4)	0.0396 (2)	
C4	0.0955 (5)	0.2500	−0.1180 (3)	0.0644 (15)	
H4C	0.0649	0.3200	−0.1066	0.077*	0.50
C5	0.2431 (5)	0.2500	−0.1451 (4)	0.0757 (18)	
H5C	0.2799	0.1810	−0.1461	0.091*	0.50
H5D	0.2517	0.2790	−0.2008	0.091*	0.50
C6	0.3879 (5)	0.0651 (3)	0.0946 (3)	0.099 (2)	
H6C	0.4498	0.0986	0.1343	0.119*	0.50
H6D	0.4220	−0.0039	0.0862	0.119*	0.50
H6E	0.4497	0.0288	0.1327	0.119*	0.50
H6F	0.3922	0.0328	0.0400	0.119*	0.50
C7	0.2450 (5)	0.0615 (3)	0.1294 (3)	0.0876 (16)	
H7C	0.1813	0.0302	0.0886	0.105*	0.50
H7D	0.2619	0.1215	0.1646	0.105*	0.50
C8	0.0056 (10)	0.2045 (7)	−0.1810 (6)	0.083 (3)	0.50

H8C	0.0391	0.1373	−0.1942	0.124*	0.50
H8D	0.0067	0.2458	−0.2307	0.124*	0.50
H8E	−0.0885	0.2001	−0.1599	0.124*	0.50
N4	0.1011 (6)	0.1921 (4)	−0.0397 (3)	0.0509 (14)	0.50
H4A	0.1155	0.1254	−0.0506	0.061*	0.50
H4B	0.0195	0.1984	−0.0117	0.061*	0.50
N5	0.3194 (6)	0.3121 (4)	−0.0839 (3)	0.0475 (14)	0.50
H5A	0.2927	0.3780	−0.0871	0.057*	0.50
H5B	0.4126	0.3082	−0.0927	0.057*	0.50
N6	0.3911 (6)	0.1202 (4)	0.0147 (3)	0.0515 (15)	0.50
H6A	0.3562	0.0811	−0.0268	0.062*	0.50
H6B	0.4796	0.1381	0.0015	0.062*	0.50
N7	0.2107 (6)	0.1694 (3)	0.1391 (4)	0.0539 (15)	0.50
H7A	0.2568	0.1949	0.1838	0.065*	0.50
H7B	0.1180	0.1763	0.1484	0.065*	0.50
C9	0.258 (3)	−0.0030 (11)	0.2011 (7)	0.073 (6)	0.42 (3)
H9C	0.3260	0.0252	0.2390	0.109*	0.42 (3)
H9D	0.2877	−0.0698	0.1837	0.109*	0.42 (3)
H9E	0.1689	−0.0080	0.2290	0.109*	0.42 (3)
N8	0.4263 (6)	0.3269 (3)	0.0947 (4)	0.0507 (14)	0.50
H8A	0.4347	0.3038	0.1478	0.061*	0.50
H8B	0.5087	0.3175	0.0681	0.061*	0.50
N9	0.1551 (6)	0.3770 (4)	0.0749 (4)	0.0532 (15)	0.50
H9A	0.1265	0.4146	0.0308	0.064*	0.50
H9B	0.0785	0.3565	0.1035	0.064*	0.50
C10	0.181 (3)	0.5209 (10)	0.174 (2)	0.086 (7)	0.38 (3)
H10A	0.2265	0.5288	0.2274	0.130*	0.38 (3)
H10B	0.0836	0.5067	0.1822	0.130*	0.38 (3)
H10C	0.1915	0.5827	0.1422	0.130*	0.38 (3)
C11	0.445 (3)	0.023 (2)	0.1699 (11)	0.138 (15)	0.20
H11A	0.5445	0.0147	0.1636	0.207*	0.20
H11B	0.4024	−0.0415	0.1811	0.207*	0.20
H11C	0.4268	0.0690	0.2158	0.207*	0.20

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0430 (4)	0.0313 (3)	0.0547 (4)	0.000	0.0079 (3)	0.000
C1	0.054 (3)	0.038 (2)	0.060 (4)	0.000	0.017 (3)	0.000
N1	0.074 (4)	0.085 (4)	0.054 (3)	0.000	0.005 (3)	0.000
C2	0.073 (3)	0.041 (2)	0.068 (3)	−0.0044 (18)	0.004 (2)	−0.0087 (18)
N2	0.152 (5)	0.0341 (18)	0.106 (4)	−0.005 (2)	−0.001 (3)	−0.0084 (19)
C3	0.040 (3)	0.061 (3)	0.065 (4)	0.000	0.012 (3)	0.000
N3	0.053 (3)	0.101 (4)	0.070 (4)	0.000	0.000 (3)	0.000
Ni2	0.0426 (4)	0.0279 (3)	0.0484 (4)	0.000	0.0071 (3)	0.000
C4	0.057 (3)	0.067 (4)	0.069 (4)	0.000	−0.006 (3)	0.000
C5	0.065 (4)	0.110 (5)	0.052 (3)	0.000	−0.002 (3)	0.000
C6	0.080 (4)	0.053 (3)	0.164 (6)	0.005 (2)	−0.028 (4)	0.043 (3)

C7	0.103 (4)	0.066 (3)	0.094 (4)	−0.021 (3)	−0.016 (3)	0.041 (3)
C8	0.067 (6)	0.099 (7)	0.082 (6)	−0.007 (5)	−0.011 (6)	−0.005 (5)
N4	0.052 (4)	0.041 (3)	0.060 (4)	0.000 (3)	0.009 (3)	0.009 (3)
N5	0.050 (3)	0.034 (3)	0.058 (4)	0.002 (2)	0.008 (3)	0.004 (3)
N6	0.052 (4)	0.032 (3)	0.071 (4)	0.001 (2)	0.008 (3)	−0.003 (3)
N7	0.049 (3)	0.053 (3)	0.059 (4)	0.005 (3)	0.005 (3)	0.007 (3)
C9	0.108 (16)	0.044 (6)	0.066 (7)	−0.002 (7)	0.019 (7)	0.018 (5)
N8	0.054 (3)	0.046 (3)	0.052 (4)	−0.002 (3)	0.014 (3)	−0.004 (3)
N9	0.055 (4)	0.036 (3)	0.068 (4)	0.001 (3)	0.017 (3)	0.000 (3)
C10	0.083 (12)	0.061 (8)	0.115 (15)	0.020 (8)	0.008 (13)	−0.006 (8)
C11	0.11 (2)	0.20 (4)	0.10 (3)	−0.07 (3)	0.032 (19)	−0.08 (3)

Geometric parameters (Å, º)

Ni1—C1	1.852 (7)	C7—C10^{i}	1.457 (7)
Ni1—C2^{i}	1.856 (4)	C7—C9	1.457 (7)
Ni1—C2	1.856 (4)	C7—N7	1.490 (3)
Ni1—C3	1.866 (7)	C7—N9^{i}	1.493 (3)
C1—N1	1.147 (7)	C7—H7C	1.0000
C2—N2	1.139 (5)	C7—H7D	1.0000
C3—N3	1.145 (8)	C8—H8C	0.9800
Ni2—N7^{i}	2.112 (6)	C8—H8D	0.9800
Ni2—N7	2.112 (6)	C8—H8E	0.9800
Ni2—N8	2.122 (6)	N4—H4A	0.9200
Ni2—N8^{i}	2.122 (6)	N4—H4B	0.9200
Ni2—N9^{i}	2.128 (6)	N5—H5A	0.9200
Ni2—N9	2.128 (6)	N5—H5B	0.9200
Ni2—N5^{i}	2.135 (6)	N6—H6A	0.9200
Ni2—N5	2.135 (6)	N6—H6B	0.9200
Ni2—N4	2.137 (6)	N7—H7A	0.9200
Ni2—N4^{i}	2.137 (6)	N7—H7B	0.9200
Ni2—N6^{i}	2.139 (5)	C9—H9C	0.9800
Ni2—N6	2.139 (5)	C9—H9D	0.9800
C4—C8	1.480 (10)	C9—H9E	0.9800
C4—N4	1.492 (3)	N8—C6^{i}	1.492 (3)
C4—C5	1.503 (6)	N8—H8A	0.9200
C4—H4C	1.0000	N8—H8B	0.9200
C5—N5	1.494 (3)	N9—C7^{i}	1.493 (3)
C5—H5C	0.9900	N9—H9A	0.9200
C5—H5D	0.9900	N9—H9B	0.9200
C6—C11	1.457 (7)	C10—C7^{i}	1.457 (7)
C6—N6	1.495 (3)	C10—H10A	0.9800
C6—C7	1.503 (6)	C10—H10B	0.9800
C6—H6C	0.9900	C10—H10C	0.9800
C6—H6D	0.9900	C11—H11A	0.9800
C6—H6E	0.9900	C11—H11B	0.9800
C6—H6F	0.9900	C11—H11C	0.9800

C1—Ni1—C2^{i}	89.46 (14)	C9—C7—C6	103.9 (11)
C1—Ni1—C2	89.46 (14)	N7—C7—C6	102.5 (4)
C2^{i}—Ni1—C2	178.9 (3)	N9^{i}—C7—C6	107.5 (4)
C1—Ni1—C3	179.7 (2)	C9—C7—H7C	109.7
C2^{i}—Ni1—C3	90.54 (14)	N7—C7—H7C	109.7
C2—Ni1—C3	90.54 (14)	C6—C7—H7C	109.7
N1—C1—Ni1	178.2 (5)	C10^{i}—C7—H7D	113.2
N2—C2—Ni1	178.6 (5)	C4—C8—H8C	109.5
N3—C3—Ni1	176.9 (5)	C4—C8—H8D	109.5
N7—Ni2—N8	92.6 (2)	H8C—C8—H8D	109.5
N7^{i}—Ni2—N8^{i}	92.6 (2)	C4—C8—H8E	109.5
N7^{i}—Ni2—N9^{i}	90.7 (2)	H8C—C8—H8E	109.5
N8^{i}—Ni2—N9^{i}	80.36 (19)	H8D—C8—H8E	109.5
N7—Ni2—N9	90.7 (2)	C4—N4—Ni2	108.0 (3)
N8—Ni2—N9	80.36 (19)	C4—N4—H4A	110.1
N8^{i}—Ni2—N5^{i}	93.3 (2)	Ni2—N4—H4A	110.1
N9^{i}—Ni2—N5^{i}	95.7 (2)	C4—N4—H4B	110.1
N8—Ni2—N5	93.3 (2)	Ni2—N4—H4B	110.1
N9—Ni2—N5	95.7 (2)	H4A—N4—H4B	108.4
N7—Ni2—N4	94.3 (2)	C5—N5—Ni2	104.8 (3)
N8—Ni2—N4	171.73 (19)	C5—N5—H5A	110.8
N9—Ni2—N4	94.9 (2)	Ni2—N5—H5A	110.8
N5—Ni2—N4	80.42 (19)	C5—N5—H5B	110.8
N7^{i}—Ni2—N4^{i}	94.3 (2)	Ni2—N5—H5B	110.8
N8^{i}—Ni2—N4^{i}	171.73 (19)	H5A—N5—H5B	108.9
N9^{i}—Ni2—N4^{i}	94.9 (2)	C6—N6—Ni2	105.7 (3)
N5^{i}—Ni2—N4^{i}	80.42 (19)	C6—N6—H6A	110.6
N7^{i}—Ni2—N6^{i}	80.95 (19)	Ni2—N6—H6A	110.6
N8^{i}—Ni2—N6^{i}	92.4 (2)	C6—N6—H6B	110.6
N9^{i}—Ni2—N6^{i}	168.7 (2)	Ni2—N6—H6B	110.6
N5^{i}—Ni2—N6^{i}	93.3 (2)	H6F—N6—H6B	108.4
N4^{i}—Ni2—N6^{i}	93.3 (2)	H6A—N6—H6B	108.7
N7—Ni2—N6	80.95 (19)	C7—N7—Ni2	110.5 (4)
N8—Ni2—N6	92.4 (2)	C7—N7—H7A	109.5
N9—Ni2—N6	168.7 (2)	Ni2—N7—H7A	109.5
N5—Ni2—N6	93.3 (2)	C7—N7—H7B	109.5
N4—Ni2—N6	93.3 (2)	Ni2—N7—H7B	109.5
C8—C4—N4	113.6 (5)	H7A—N7—H7B	108.1
C8—C4—C5	111.2 (5)	C7—C9—H9C	109.5
N4—C4—C5	102.5 (4)	C7—C9—H9D	109.5
C8—C4—H4C	109.8	C7—C9—H9E	109.5
N4—C4—H4C	109.8	C6^{i}—N8—Ni2	106.6 (4)
C5—C4—H4C	109.8	C6^{i}—N8—H8A	110.4
N5—C5—C4	106.2 (4)	Ni2—N8—H8A	110.4
N5—C5—H5C	110.5	C6^{i}—N8—H8B	110.4
C4—C5—H5C	110.5	Ni2—N8—H8B	110.4
N5—C5—H5D	110.5	H8A—N8—H8B	108.6
C4—C5—H5D	110.5	C7^{i}—N9—Ni2	109.5 (3)

H5C—C5—H5D	108.7	C7^{i}—N9—H9A	109.8
C11—C6—N6	155.9 (13)	Ni2—N9—H9A	109.8
C11—C6—C7	91.4 (13)	C7^{i}—N9—H9B	109.8
N6—C6—C7	111.3 (4)	Ni2—N9—H9B	109.8
N6—C6—H6C	109.4	H9A—N9—H9B	108.2
C7—C6—H6C	109.4	C7^{i}—C10—H10A	109.5
N6—C6—H6D	109.4	C7^{i}—C10—H10B	109.5
C7—C6—H6D	109.4	H10A—C10—H10B	109.5
H6C—C6—H6D	108.0	C7^{i}—C10—H10C	109.5
C7—C6—H6E	108.1	H10A—C10—H10C	109.5
C7—C6—H6F	111.3	H10B—C10—H10C	109.5
H6E—C6—H6F	108.8	C6—C11—H11A	109.5
C9—C7—N7	120.5 (7)	C6—C11—H11B	109.5
C10^{i}—C7—N9^{i}	117.6 (14)	H6E—C11—H11B	108.6
C10^{i}—C7—C6	127.2 (9)	C6—C11—H11C	109.5

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···N2^{ii}	0.92	2.24	3.140 (7)	167
N5—H5*A*···N2^{iii}	0.92	2.17	3.083 (6)	169
N5—H5*B*···N3	0.92	2.30	3.180 (8)	159
N6—H6*A*···N2^{ii}	0.92	2.23	3.073 (7)	152
N6—H6*B*···N3	0.92	2.54	3.349 (7)	147
N7—H7*A*···N1^{iv}	0.92	2.42	3.295 (8)	158
N7—H7*B*···N1^{v}	0.92	2.36	3.159 (7)	145
N8—H8*A*···N1^{iv}	0.92	2.07	2.985 (8)	179
N9—H9*A*···N2^{iii}	0.92	2.42	3.212 (8)	144

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