

# Tris(propane-1,2-diamine- $\kappa^2N,N'$ )-nickel(II) tetracyanidoplatinate(II)

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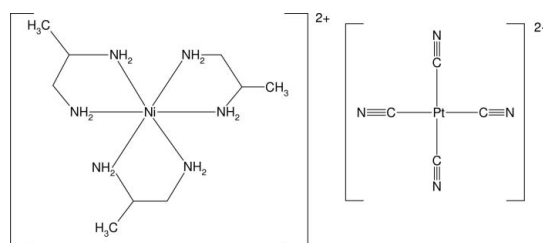
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Key indicators: single-crystal X-ray study;  $T = 220$  K; mean  $\sigma(\text{C}-\text{C}) = 0.015$  Å; disorder in main residue;  $R$  factor = 0.034;  $wR$  factor = 0.084; data-to-parameter ratio = 13.7.

In the title compound,  $[\text{Ni}(\text{C}_3\text{H}_{10}\text{N}_2)_3][\text{Pt}(\text{CN})_4]$ , the  $[\text{Pt}(\text{CN})_4]^{2-}$  anion with the environment of the  $\text{Pt}^{\text{II}}$  atom, lying on a mirror plane, is square planar, whereas the  $\text{Ni}^{\text{II}}$  atom in the  $[\text{Ni}(\text{C}_3\text{N}_2\text{H}_{10})_3]^{2+}$  cation, also lying on a mirror plane, has a slightly distorted octahedral coordination geometry. Three chiral 1,2-diaminopropane molecules, which are disordered equally over two sets of positions, adopt  $\Delta(\delta\delta\delta)$  and  $\Delta(\lambda\lambda\lambda)$  configurations. The average Ni–N and Pt–C bond lengths are 2.131 (10) and 1.988 (10) Å, respectively. The cations and anions are connected by  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds.

## Related literature

For related literature on compounds with  $[\text{Ni}(1,2\text{-diaminopropane})_3]^{2+}$  cations, see: Behrens *et al.* (2003) for  $\text{Sn}_2\text{S}_6^{4-}$ ; Kuchár & Černák (2008) for  $[\text{Ni}(\text{CN})_4]^{2-}$ ; Lin *et al.* (2005) for  $[\text{H}_3\text{Ge}_{14}\text{NiO}_{27}]^{4-}$ ; Nasanen *et al.* (1964) for  $\text{ClO}_4^-$ ; Saha *et al.* (2005) for  $[\text{Fe}(\text{CN})_5\text{NO}]^{2-}$ .



## Experimental

### Crystal data

$[\text{Ni}(\text{C}_3\text{H}_{10}\text{N}_2)_3][\text{Pt}(\text{CN})_4]$   
 $M_r = 580.27$

Orthorhombic,  $Pnma$   
 $a = 9.8206$  (18) Å

$b = 13.694$  (2) Å  
 $c = 16.261$  (3) Å  
 $V = 2186.8$  (7) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 7.27$  mm<sup>-1</sup>  
 $T = 220$  K  
 $0.38 \times 0.11 \times 0.06$  mm

### Data collection

Stoe IPDS diffractometer  
Absorption correction: numerical  
(*IPDS FACE*; Stoe & Cie, 1999)  
 $T_{\text{min}} = 0.104$ ,  $T_{\text{max}} = 0.446$

15408 measured reflections  
2197 independent reflections  
1807 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.088$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$   
 $wR(F^2) = 0.085$   
 $S = 1.04$   
2197 reflections

160 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 1.23$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -1.92$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Pt–C1	1.958 (10)	Ni–N30	2.122 (10)
Pt–C2	1.995 (11)	Ni–N40	2.137 (9)
Pt–C3	1.999 (9)	Ni–N11 <sup>i</sup>	2.142 (10)
Ni–N21 <sup>i</sup>	2.118 (9)	Ni–N20	2.142 (10)
Ni–N10	2.127 (9)		
C1–Pt–C2	179.4 (3)	N21 <sup>i</sup> –Ni–N11 <sup>i</sup>	80.5 (4)
C1–Pt–C3	89.5 (2)	N10–Ni–N11 <sup>i</sup>	93.3 (4)
C2–Pt–C3	90.5 (2)	N30–Ni–N11 <sup>i</sup>	94.4 (4)
C3 <sup>i</sup> –Pt–C3	178.8 (4)	N40–Ni–N11 <sup>i</sup>	170.6 (4)
N21 <sup>i</sup> –Ni–N10	171.3 (4)	N21 <sup>i</sup> –Ni–N20	93.8 (4)
N21 <sup>i</sup> –Ni–N30	93.3 (4)	N10–Ni–N20	80.4 (4)
N10–Ni–N30	93.3 (4)	N30–Ni–N20	170.1 (4)
N21 <sup>i</sup> –Ni–N40	91.7 (4)	N40–Ni–N20	92.2 (4)
N10–Ni–N40	95.0 (4)	N11 <sup>i</sup> –Ni–N20	93.5 (4)
N30–Ni–N40	80.8 (4)		

Symmetry code: (i)  $x, -y + \frac{1}{2}, z$ .

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N21–H21F <sup>·</sup> ··N2	0.90	2.51	3.311 (12)	148
N40–H40A <sup>·</sup> ··N2	0.90	2.30	3.160 (14)	160
N10–H10B <sup>·</sup> ··N3 <sup>ii</sup>	0.90	2.40	3.193 (13)	148
N21–H21E <sup>·</sup> ··N3 <sup>ii</sup>	0.90	2.24	3.066 (13)	152
N40–H40B <sup>·</sup> ··N3 <sup>ii</sup>	0.90	2.21	3.098 (12)	169
N11–H11C <sup>·</sup> ··N1 <sup>iii</sup>	0.90	2.48	3.342 (13)	159
N20–H20B <sup>·</sup> ··N1 <sup>iii</sup>	0.90	2.11	3.005 (12)	174
N11–H11D <sup>·</sup> ··N1 <sup>iv</sup>	0.90	2.46	3.242 (13)	145
N30–H30B <sup>·</sup> ··N3 <sup>v</sup>	0.90	2.31	3.191 (11)	166

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

Data collection: *IPDS EXPOSE* (Stoe & Cie, 1999); cell refinement: *IPDS CELL* (Stoe & Cie, 1999); data reduction: *IPDS INTEGRATE* (Stoe & Cie, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2111).

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**supplementary materials**

*Acta Cryst.* (2008). E64, m235-m236 [ doi:10.1107/S1600536807066913 ]

## Tris(propane-1,2-diamine- $\kappa^2N,N'$ )nickel(II) tetracyanidoplatinate(II)

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### Comment

The title compound,  $[\text{Ni}(\text{pn})_3][\text{Pt}(\text{CN})_4]$  (pn = 1,2-diaminopropane) has been prepared by a chance within our studies on the role of hydrogen bonds as possible exchange paths for magnetic interactions in low-dimensional compounds. The compound consists of discrete  $[\text{Ni}(\text{pn})_3]^{2+}$  cations and  $[\text{Pt}(\text{CN})_4]^{2-}$  anions (Fig. 1). Selected bond lengths and angles are given in Table 1. The  $\text{Ni}^{\text{II}}$  atom is coordinated by six N atoms of three racemic pn ligands, which are disordered over two sets of positions, with site occupancies of 0.50 (except methylene and methine C atoms), thus forming  $\Delta(\delta\delta\delta)$  and  $\Delta(\lambda\lambda\lambda)$  configurations. Moreover, a mirror plane passes through the tetracyanoplatinate anion (N1, C1, Pt, C2 and N2 atoms) and the  $[\text{Ni}(\text{pn})_3]^{2+}$  cation (Ni, C31 and C41 atoms). The coordination geometry around the  $\text{Ni}^{\text{II}}$  atom can be described as octahedral. The two N atoms occupying axial positions form an angle of  $170.6(4)^\circ$  and the Ni—N bond distances range from 2.118(9)–2.142(10) Å [mean bond length is 2.131(10) Å], in good agreement with the values reported of other  $[\text{Ni}(\text{pn})_3]^{2+}$  complexes (Behrens *et al.*, 2003; Kuchár & Černák, 2008; Saha *et al.*, 2005). Octahedral coordination geometry around the Ni atom was observed also in other compounds with  $[\text{Ni}(\text{pn})_3]^{2+}$  cation (Nasanen *et al.*, 1964; Lin *et al.*, 2005). The square-planar geometry of  $[\text{Pt}(\text{CN})_4]^{2-}$  is in good agreement with those of the previous studies with average Pt—C bond lengths of 1.988(10) Å. The structure is stabilized also by the N—H $\cdots$ N hydrogen bonds between the cations and anions (Table 2).

### Experimental

The title compound were prepared by a chance during our attempts to prepare chain-like  $[\text{Ni}(\text{pn})_2][\text{Pt}(\text{CN})_4]$  compound suitable for magnetic studies. A mixture of a 10 ml aqueous solution of  $\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$  (0.132 g, 0.5 mmol) and pn (0.086 ml, 1.0 mmol) was stirred for 30 min and a 10 ml aqueous solution of  $\text{K}_2[\text{Pt}(\text{CN})_4] \cdot 3\text{H}_2\text{O}$  (0.216 g, 0.5 mmol) was added. The pink precipitate thus formed was dissolved by addition of a concentrated solution of ammonia (20 ml). After few days, pink crystals of the title compound were filtered off and dried in air.

### Refinement

H atoms were positioned geometrically and refined as riding atoms, with N—H = 0.90 Å, C—H = 0.97 Å ( $\text{CH}_2$ ), 0.98 Å ( $\text{CH}$ ) and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$  and with C—H = 0.96 Å ( $\text{CH}_3$ ) and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ . The highest residual electron density and the deepest hole were found 1.01 and 0.88 Å from the Pt atom, respectively.

## Figures

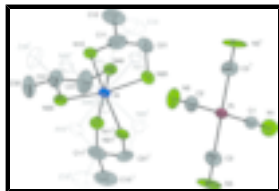


Fig. 1. The structures of the cation and anion in the title compound. Displacement ellipsoids are drawn at the 40% probability level. Coloured atoms and black bonds show the  $\Delta(\delta\delta\delta)$  configuration whereas transparent atoms and bonds represent the  $\Delta(\lambda\lambda\lambda)$  configuration of the  $[\text{Ni}(\text{pn})_3]^{2+}$  cation. Hydrogen atoms are omitted for clarity. [Symmetry code: (i)  $x, 1/2 - y, z.$ ]

## Tris(propane-1,2-diamine- $\kappa^2N,N'$ )nickel(II) tetracyanidoplatinate(II)

### Crystal data

$[\text{Ni}(\text{C}_3\text{H}_{10}\text{N}_2)_3][\text{Pt}(\text{CN})_4]$

$M_r = 580.27$

Orthorhombic,  $Pnma$

Hall symbol:  $-P\ 2ac\ 2n$

$a = 9.8206$  (18) Å

$b = 13.694$  (2) Å

$c = 16.261$  (3) Å

$V = 2186.8$  (7) Å<sup>3</sup>

$Z = 4$

$F_{000} = 1136$

$D_x = 1.762$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 8000 reflections

$\theta = 2.4\text{--}25.9^\circ$

$\mu = 7.27$  mm<sup>-1</sup>

$T = 220$  K

Needle, pink

$0.38 \times 0.11 \times 0.06$  mm

### Data collection

Stoe IPDS  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 220$  K

$\varphi$  scans

Absorption correction: numerical  
(IPDS FACE; Stoe & Cie, 1999)

$T_{\min} = 0.104, T_{\max} = 0.446$

15408 measured reflections

2197 independent reflections

1807 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.088$

$\theta_{\max} = 25.9^\circ$

$\theta_{\min} = 2.4^\circ$

$h = -12 \rightarrow 12$

$k = -16 \rightarrow 16$

$l = -19 \rightarrow 19$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.085$

$S = 1.04$

2197 reflections

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.23$  e Å<sup>-3</sup>

160 parameters

$$\Delta\rho_{\min} = -1.92 \text{ e } \text{\AA}^{-3}$$

Primary atom site location: structure-invariant direct methods

Extinction correction: none

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Pt	0.20444 (3)	0.2500	0.07418 (2)	0.04021 (13)	
Ni	0.73154 (10)	0.2500	0.02973 (6)	0.0368 (2)	
C1	0.1023 (9)	0.2500	0.1776 (5)	0.0475 (19)	
N1	0.0397 (9)	0.2500	0.2376 (5)	0.072 (2)	
C2	0.3067 (9)	0.2500	-0.0318 (7)	0.058 (2)	
N2	0.3700 (10)	0.2500	-0.0916 (6)	0.079 (3)	
C3	0.2044 (8)	0.1040 (6)	0.0754 (5)	0.069 (2)	
N3	0.2032 (10)	0.0220 (4)	0.0777 (5)	0.106 (3)	
C21	0.6124 (10)	0.4305 (6)	0.0987 (7)	0.104 (3)	
H21A	0.5531	0.4642	0.1370	0.124*	0.50
H21B	0.6074	0.4631	0.0458	0.124*	0.50
H21C	0.5802	0.4971	0.0931	0.124*	0.50
H21D	0.5536	0.3967	0.1372	0.124*	0.50
N10	0.8434 (11)	0.3735 (7)	0.0711 (6)	0.048 (2)	0.50
H10A	0.9198	0.3542	0.0970	0.058*	0.50
H10B	0.8672	0.4112	0.0281	0.058*	0.50
N20	0.5722 (11)	0.3283 (7)	0.0909 (6)	0.051 (2)	0.50
H20A	0.4945	0.3238	0.0617	0.062*	0.50
H20B	0.5575	0.3024	0.1410	0.062*	0.50
C11	0.7537 (11)	0.4303 (6)	0.1294 (6)	0.085 (3)	
H11A	0.7449	0.3821	0.1737	0.101*	0.50
H11B	0.8156	0.4621	0.0905	0.101*	0.50
N11	0.7811 (10)	0.3348 (8)	0.1363 (6)	0.051 (3)	0.50
H11C	0.7346	0.3108	0.1795	0.061*	0.50
H11D	0.8704	0.3275	0.1471	0.061*	0.50
N21	0.6087 (10)	0.3743 (6)	0.0070 (6)	0.048 (2)	0.50
H21E	0.6445	0.4121	-0.0328	0.057*	0.50
H21F	0.5234	0.3572	-0.0071	0.057*	0.50
C31	0.9053 (10)	0.2500	-0.1186 (6)	0.067 (3)	
H31	0.9357	0.3170	-0.1082	0.081*	0.50
C41	0.7596 (13)	0.2500	-0.1515 (6)	0.087 (4)	
H41A	0.7236	0.1841	-0.1547	0.104*	0.50
H41B	0.7551	0.2798	-0.2056	0.104*	0.50
N30	0.8963 (10)	0.1956 (7)	-0.0412 (6)	0.047 (2)	0.50
H30A	0.9746	0.2020	-0.0128	0.056*	0.50
H30B	0.8835	0.1317	-0.0517	0.056*	0.50
N40	0.6798 (11)	0.3121 (7)	-0.0867 (6)	0.047 (2)	0.50
H40A	0.5895	0.3084	-0.0956	0.057*	0.50
H40B	0.7054	0.3752	-0.0890	0.057*	0.50
C32	0.9945 (15)	0.2029 (13)	-0.1810 (9)	0.089 (5)	0.50
H32A	1.0867	0.2023	-0.1615	0.134*	0.50

## supplementary materials

H32B	0.9898	0.2389	-0.2316	0.134*	0.50
H32C	0.9644	0.1371	-0.1903	0.134*	0.50
C12	0.808 (3)	0.5133 (17)	0.1769 (16)	0.101 (7)	0.50
H12A	0.9003	0.5003	0.1922	0.151*	0.50
H12B	0.7537	0.5224	0.2255	0.151*	0.50
H12C	0.8041	0.5714	0.1438	0.151*	0.50
C13	0.721 (3)	0.4965 (18)	0.2020 (17)	0.101 (7)	0.50
H13A	0.8029	0.5079	0.2332	0.151*	0.50
H13B	0.6546	0.4658	0.2364	0.151*	0.50
H13C	0.6867	0.5576	0.1821	0.151*	0.50

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Pt	0.0384 (2)	0.02827 (17)	0.0540 (2)	0.000	-0.00989 (13)	0.000
Ni	0.0390 (5)	0.0239 (5)	0.0476 (5)	0.000	-0.0062 (4)	0.000
C1	0.048 (5)	0.040 (4)	0.055 (5)	0.000	-0.006 (4)	0.000
N1	0.073 (6)	0.080 (7)	0.064 (5)	0.000	-0.008 (5)	0.000
C2	0.041 (5)	0.064 (6)	0.068 (6)	0.000	-0.013 (5)	0.000
N2	0.048 (5)	0.117 (9)	0.072 (6)	0.000	0.005 (4)	0.000
C3	0.076 (6)	0.057 (5)	0.074 (4)	0.005 (4)	0.001 (4)	-0.007 (4)
N3	0.177 (11)	0.016 (3)	0.124 (6)	0.004 (4)	0.013 (5)	-0.014 (3)
C21	0.080 (6)	0.044 (4)	0.187 (10)	0.005 (4)	0.037 (7)	-0.042 (5)
N10	0.044 (6)	0.033 (5)	0.066 (6)	-0.005 (4)	-0.014 (5)	-0.007 (5)
N20	0.050 (6)	0.046 (5)	0.057 (6)	0.007 (5)	-0.007 (5)	-0.005 (4)
C11	0.104 (6)	0.053 (5)	0.097 (6)	-0.021 (5)	0.015 (5)	-0.033 (4)
N11	0.053 (7)	0.045 (6)	0.053 (5)	0.000 (5)	-0.008 (5)	-0.003 (5)
N21	0.047 (5)	0.026 (4)	0.070 (6)	-0.002 (4)	-0.015 (5)	-0.001 (4)
C31	0.055 (6)	0.085 (8)	0.063 (6)	0.000	0.007 (5)	0.000
C41	0.065 (6)	0.153 (13)	0.043 (5)	0.000	0.006 (5)	0.000
N30	0.047 (6)	0.035 (5)	0.058 (5)	-0.002 (4)	-0.011 (4)	0.005 (4)
N40	0.046 (5)	0.036 (5)	0.059 (6)	-0.001 (4)	-0.013 (4)	0.007 (4)
C32	0.054 (8)	0.124 (15)	0.091 (10)	0.021 (9)	0.018 (8)	-0.005 (9)
C12	0.14 (2)	0.057 (9)	0.110 (14)	0.000 (12)	-0.024 (13)	-0.020 (9)
C13	0.14 (2)	0.057 (9)	0.110 (14)	0.000 (12)	-0.024 (13)	-0.020 (9)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Pt—C1	1.958 (10)	N20—H20B	0.9000
Pt—C2	1.995 (11)	C11—N11	1.340 (13)
Pt—C3 <sup>i</sup>	1.999 (9)	C11—C13	1.52 (3)
Pt—C3	1.999 (9)	C11—C12	1.47 (2)
Ni—N21 <sup>i</sup>	2.118 (9)	C11—H11A	0.9800
Ni—N21	2.118 (9)	C11—H11B	0.9800
Ni—N10	2.127 (9)	N11—H11C	0.9000
Ni—N10 <sup>i</sup>	2.127 (9)	N11—H11D	0.9000
Ni—N30 <sup>i</sup>	2.122 (10)	N21—H21E	0.9000
Ni—N30	2.122 (10)	N21—H21F	0.9000

Ni—N40 <sup>i</sup>	2.137 (9)	C31—N30	1.466 (12)
Ni—N40	2.137 (9)	C31—C32	1.487 (16)
Ni—N11	2.142 (10)	C31—C41	1.528 (16)
Ni—N11 <sup>i</sup>	2.142 (10)	C31—H31	0.9800
Ni—N20	2.142 (10)	C41—N40	1.565 (13)
Ni—N20 <sup>i</sup>	2.142 (10)	C41—H41A	0.9700
C1—N1	1.154 (11)	C41—H41B	0.9700
C2—N2	1.154 (13)	N30—H30A	0.9000
C3—N3	1.124 (11)	N30—H30B	0.9000
C21—N20	1.460 (13)	N40—H40A	0.9000
C21—C11	1.474 (14)	N40—H40B	0.9000
C21—N21	1.679 (13)	C32—H32A	0.9600
C21—H21A	0.9700	C32—H32B	0.9600
C21—H21B	0.9700	C32—H32C	0.9600
C21—H21C	0.9700	C12—H12A	0.9600
C21—H21D	0.9700	C12—H12B	0.9600
N10—C11	1.509 (14)	C12—H12C	0.9600
N10—H10A	0.9000	C13—H13A	0.9600
N10—H10B	0.9000	C13—H13B	0.9600
N20—H20A	0.9000	C13—H13C	0.9600
C1—Pt—C2	179.4 (3)	N11—C11—C13	124.0 (13)
C1—Pt—C3 <sup>i</sup>	89.5 (2)	C21—C11—C13	93.8 (12)
C2—Pt—C3 <sup>i</sup>	90.5 (2)	C21—C11—C12	120.9 (13)
C1—Pt—C3	89.5 (2)	N10—C11—C12	121.1 (13)
C2—Pt—C3	90.5 (2)	C21—C11—H11A	99.6
C3 <sup>i</sup> —Pt—C3	178.8 (4)	N10—C11—H11A	99.6
N21 <sup>i</sup> —Ni—N10	171.3 (4)	C12—C11—H11A	99.6
N21—Ni—N10 <sup>i</sup>	171.3 (4)	N11—C11—H11B	111.4
N21—Ni—N30 <sup>i</sup>	93.3 (4)	C21—C11—H11B	111.4
N10 <sup>i</sup> —Ni—N30 <sup>i</sup>	93.3 (4)	C13—C11—H11B	111.4
N21 <sup>i</sup> —Ni—N30	93.3 (4)	C11—N11—Ni	114.6 (7)
N10—Ni—N30	93.3 (4)	C11—N11—H11C	108.6
N21—Ni—N40 <sup>i</sup>	91.7 (4)	Ni—N11—H11C	108.6
N10 <sup>i</sup> —Ni—N40 <sup>i</sup>	95.0 (4)	C11—N11—H11D	108.6
N30 <sup>i</sup> —Ni—N40 <sup>i</sup>	80.8 (4)	Ni—N11—H11D	108.6
N21 <sup>i</sup> —Ni—N40	91.7 (4)	H11C—N11—H11D	107.6
N10—Ni—N40	95.0 (4)	C21—N21—Ni	101.6 (6)
N30—Ni—N40	80.8 (4)	C21—N21—H21E	111.5
N21—Ni—N11	80.5 (4)	Ni—N21—H21E	111.5
N10 <sup>i</sup> —Ni—N11	93.3 (4)	C21—N21—H21F	111.5
N30 <sup>i</sup> —Ni—N11	94.4 (4)	Ni—N21—H21F	111.5
N40 <sup>i</sup> —Ni—N11	170.6 (4)	H21E—N21—H21F	109.3
N21 <sup>i</sup> —Ni—N11 <sup>i</sup>	80.5 (4)	N30—C31—C32	113.6 (8)
N10—Ni—N11 <sup>i</sup>	93.3 (4)	N30—C31—C41	104.1 (7)



## supplementary materials

N30—Ni—N11 <sup>i</sup>	94.4 (4)	C32—C31—C41	108.2 (9)
N40—Ni—N11 <sup>i</sup>	170.6 (4)	N30—C31—H31	110.2
N21 <sup>i</sup> —Ni—N20	93.8 (4)	C32—C31—H31	110.2
N10—Ni—N20	80.4 (4)	C41—C31—H31	110.2
N30—Ni—N20	170.1 (4)	C31—C41—N40	103.5 (7)
N40—Ni—N20	92.2 (4)	C31—C41—H41A	111.1
N11 <sup>i</sup> —Ni—N20	93.5 (4)	N40—C41—H41A	111.1
N21—Ni—N20 <sup>i</sup>	93.8 (4)	C31—C41—H41B	111.1
N10 <sup>i</sup> —Ni—N20 <sup>i</sup>	80.4 (4)	N40—C41—H41B	111.1
N30 <sup>i</sup> —Ni—N20 <sup>i</sup>	170.1 (4)	H41A—C41—H41B	109.0
N40 <sup>i</sup> —Ni—N20 <sup>i</sup>	92.2 (4)	C31—N30—Ni	109.5 (6)
N11—Ni—N20 <sup>i</sup>	93.5 (4)	C31—N30—H30A	109.8
N1—C1—Pt	178.6 (8)	Ni—N30—H30A	109.8
N2—C2—Pt	177.6 (8)	C31—N30—H30B	109.8
N3—C3—Pt	178.5 (8)	Ni—N30—H30B	109.8
N20—C21—C11	106.4 (8)	H30A—N30—H30B	108.2
C11—C21—N21	108.7 (7)	C41—N40—Ni	105.2 (6)
N20—C21—H21A	110.4	C41—N40—H40A	110.7
C11—C21—H21A	110.4	Ni—N40—H40A	110.7
N20—C21—H21B	110.4	C41—N40—H40B	110.7
C11—C21—H21B	110.4	Ni—N40—H40B	110.7
H21A—C21—H21B	108.6	H40A—N40—H40B	108.8
C11—C21—H21C	110.0	C31—C32—H32A	109.5
N21—C21—H21C	110.0	C31—C32—H32B	109.5
C11—C21—H21D	110.0	H32A—C32—H32B	109.5
N21—C21—H21D	110.0	C31—C32—H32C	109.5
H21C—C21—H21D	108.3	H32A—C32—H32C	109.5
C11—N10—Ni	107.8 (7)	H32B—C32—H32C	109.5
C11—N10—H10A	110.1	C11—C12—H12A	109.5
Ni—N10—H10A	110.1	C11—C12—H12B	109.5
C11—N10—H10B	110.1	H12A—C12—H12B	109.5
Ni—N10—H10B	110.1	C11—C12—H12C	109.5
H10A—N10—H10B	108.5	H12A—C12—H12C	109.5
C21—N20—Ni	108.8 (7)	H12B—C12—H12C	109.5
C21—N20—H20A	109.9	C11—C13—H13A	109.5
Ni—N20—H20A	109.9	C11—C13—H13B	109.5
C21—N20—H20B	109.9	H13A—C13—H13B	109.5
Ni—N20—H20B	109.9	C11—C13—H13C	109.5
H20A—N20—H20B	108.3	H13A—C13—H13C	109.5
N11—C11—C21	102.7 (8)	H13B—C13—H13C	109.5
C21—C11—N10	109.7 (7)		

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

### Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N21—H21F $\cdots$ N2	0.90	2.51	3.311 (12)	148

N40—H40A···N2	0.90	2.30	3.160 (14)	160
N10—H10B···N3 <sup>ii</sup>	0.90	2.40	3.193 (13)	148
N21—H21E···N3 <sup>ii</sup>	0.90	2.24	3.066 (13)	152
N40—H40B···N3 <sup>ii</sup>	0.90	2.21	3.098 (12)	169
N11—H11C···N1 <sup>iii</sup>	0.90	2.48	3.342 (13)	159
N20—H20B···N1 <sup>iii</sup>	0.90	2.11	3.005 (12)	174
N11—H11D···N1 <sup>iv</sup>	0.90	2.46	3.242 (13)	145
N30—H30B···N3 <sup>v</sup>	0.90	2.31	3.191 (11)	166

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

Fig. 1

