Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

cis-Bis(tricyanomethanido-κN)[tris(2-aminoethyl)amine-$\kappa^4 N$]nickel(II)

Ivan Potočňák,[a] Gábor Lancz,[a] Aleš Růžička[b] and Lothar Jäger[c]*

[a]Institute of Chemistry, Faculty of Science, P. J. Šafárik University, Moyzesova 11, SK-041 54 Košice, Slovakia, [b]Department of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, Čs. legií 565 Square, CZ-532 10 Pardubice, Czech Republic, and [c]Institute of Inorganic Chemistry, Martin-Luther-Universität, Halle–Wittenberg, Kurt-Mothes-Strasse 2, D-06120 Halle, Germany
Correspondence e-mail: ivan.potocnak@upjs.sk

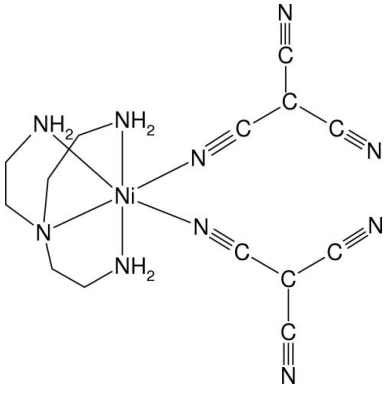
Received 25 June 2007; accepted 28 June 2007

Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.006 Å; R factor = 0.041; wR factor = 0.091; data-to-parameter ratio = 15.5.

The crystal structure of the title complex, $[Ni(C_4N_3)_2(C_6H_{18}N_4)]$, is made up of neutral mononuclear $[Ni(tren)\{C(CN)_3\}_2]$ units [tren = tris(2-aminoethyl)amine] which are linked through van der Waals interactions and N—H···N hydrogen bonds. The Ni atom has a distorted octahedral coordination environment, bonded to the four tren N atoms [average Ni—N = 2.096 (17) Å] and the two *cis*-positioned $C(CN)_3$ N atoms [Ni—N = 2.045 (4) and 2.118 (4) Å].

Related literature

For related $[Ni(tren)X_2]$ complexes, see: $X = N(CN)_2$ (Březina *et al.*, 1999); $X = NO_2$ (Wen *et al.*, 1998); X = NCS (Santarsiero & Schomaker, 1983; Rasmussen, 1959).



Experimental

Crystal data

$[Ni(C_4N_3)_2(C_6H_{18}N_4)]$
M_r = 385.07
Orthorhombic, $P2_12_12$
a = 14.4376 (11) Å
b = 15.2861 (12) Å
c = 8.0888 (6) Å
V = 1785.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.11 mm^{-1}
T = 150 (1) K
0.47 × 0.44 × 0.39 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: Gaussian integration (Coppens, 1970)
T_{min} = 0.589, T_{max} = 0.672
12191 measured reflections
3504 independent reflections
2761 reflections with $I > 2\sigma(I)$
R_{int} = 0.077

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.091
S = 1.10
3504 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}
Absolute structure: Flack (1983), with 1487 Friedel pairs
Flack parameter: −0.005 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
N30—H30A···N6^{i}	0.90	2.27	3.119 (5)	158
N30—H30B···N5^{ii}	0.90	2.32	3.141 (4)	152
N20—H20A···N3^{iii}	0.90	2.22	3.090 (5)	164
N20—H20B···N3^{iv}	0.90	2.53	3.347 (5)	151
N10—H10A···N2^{v}	0.90	2.38	3.183 (6)	149
N10—H10B···N5^{vi}	0.90	2.38	3.090 (5)	136

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

Data collection: *COLLECT* (Nonius, 1998) and *DENZO* (Otwinowski & Minor, 1997); cell refinement: *COLLECT* and *DENZO*; data reduction: *COLLECT* and *DENZO*; 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*.

This work was supported by the Slovak Grant Agency VEGA (grant No. 1/2470/05) and by APVV (grant No. 20–005204).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2024).

References

Brandenburg, K. (2001). *DIAMOND*. Release 2.1e. Crystal Impact GbR, Bonn, Germany.
Březina, F., Trávníček, Z., Šindelář, Z., Pastorek, R. & Marek, J. (1999). *Transition Met. Chem.* **24**, 459–462.
Coppens, P. (1970). *Crystallographic Computing*, edited by F. R. Ahmed, S. R. Hall & C. P. Huber, pp. 255–270. Copenhagen: Munksgaard.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.

  doi:10.1107/S1600536807031807

Rasmussen, S. E. (1959). *Acta Chem. Scand.* **13**, 2009–2022.
Santarsiero, B. D. & Schomaker, V. (1983). *Acta Cryst.* C**39**, 1216–1217.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wen, R., Bernal, I., Somoza, F., Li, W. & Fronczek, F. R. (1998). *Inorg. Chim. Acta*, **282**, 96–109.

supplementary materials

Acta Cryst. (2007). E**63**, m2072-m2073 [**doi:10.1107/S1600536807031807**]

cis-Bis(tricyanomethanido-κN)[tris(2-aminoethyl)amine-$\kappa^4 N$]nickel(II)

I. Potocnák, G. Lancz, A. Ruzicka and L. Jäger

Comment

The title compound [Ni(tren){C(CN)$_3$}$_2$] (I) has been prepared by a chance during our attempts to prepare compounds suitable for magnetic studies containing a binuclear [Ni(tren)-μ-{C(CN)$_3$}$_2$(tren)Ni]$^{2+}$ cation. The structure of (I) is made up of neutral [Ni(tren){C(CN)$_3$}$_2$] mononuclear units (Fig. 1). The nickel atom is six-coordinated: six nitrogen atoms from a tetradentate tren ligand and from two monodentate C(CN)$_3$ anionic ligands form a distorted octahedron around the metal atom. The Ni—N(tren) bond lengths [2.096 (17) Å on average] are very close to that of Ni—N(tren) found in other [Ni(tren)X_2] complexes with NiN$_6$ chromophore, where *X* is N(CN)$_2$ [2.11 (3) Å] (Březina *et al.*, 1999), *X* is NO$_2$ [2.10 (3) Å] (Wen *et al.*, 1998) and *X* is NCS [2.12 (3) Å] (Santarsiero & Schomaker, 1983) but are shorter than in the first report on this structure [2.18 (5) Å] (Rasmussen, 1959). The N4—Ni1—N1 angle which involves nitrogen atoms from two C(CN)$_3$ anions is nearly 90° but the angles around the nickel atom involving at least one nitrogen atom from the tren are much more deviated from the ideal values because of steric hindrances within the tren ligand.

The molecules of (I) are linked through van der Waals interactions and N—H···N hydrogen bonds involving all amine hydrogen atoms and uncoordinated nitrogen atoms of C(CN)$_3$; those with an N—H···N angle greater than 120° and an H···N distance less than 2.6 Å are given in Table. Through these hydrogen bonds, molecules are interconnected to form a three-dimensional structure as shown in Fig. 2.

Experimental

The title compound [Ni(tren){C(CN)$_3$}$_2$] (I) has been prepared by a chance during our attempts to prepare compounds suitable for magnetic studies containing a binuclear [Ni(tren)-μ-{C(CN)$_3$}$_2$(tren)Ni]$^{2+}$ cation. Crystals of (I) were prepared by mixing a 0.1 *M* aqueous solution of NiSO$_4$ (5 ml) with a 0.45 *M* aqueous solution of tren (1.2 ml). To the resulting violet solution, 64.6 mg of KC(CN)$_3$ (0.5 mmol) in 20 ml of water was added. Red-violet crystals of (I) appeared after 1 week. The crystals suitable for X-ray analysis were recrystallized from water and were filtered off and dried in air.

Refinement

The structure was solved by direct method and subsequent Fourier syntheses. 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 than temperature factors of their parent carbon atoms.

Figures

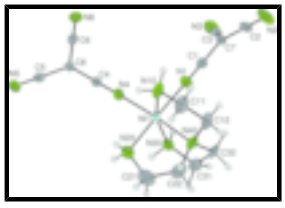


Fig. 1. The structure of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 40% probability level and H atoms are shown as small spheres of arbitrary radii.

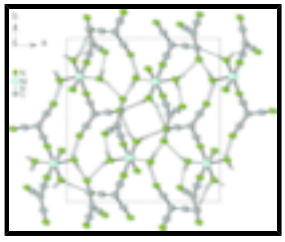


Fig. 2. Hydrogen bond system (dashed lines) in (I) viewed along the *c* axis. Methylene groups from the tren ligand are omitted because of clarity.

cis-Bis(tricyanomethanido-κ*N*)[tris(2-aminoethyl)amine-κ^4*N*]nickel(II))

Crystal data

$[Ni(C_4N_3)_2(C_6H_{18}N_4)]$	F_{000} = 800
M_r = 385.07	D_x = 1.433 Mg m^{-3}
Orthorhombic, $P2_12_12$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2 2ab	Cell parameters from 13020 reflections
a = 14.4376 (11) Å	θ = 1–27.5º
b = 15.2861 (12) Å	μ = 1.11 mm^{-1}
c = 8.0888 (6) Å	T = 150 (1) K
V = 1785.2 (2) Å^3	Block, red-violet
Z = 4	0.47 × 0.44 × 0.39 mm

Data collection

Nonius KappaCCD area-detector diffractometer	3504 independent reflections
Radiation source: fine-focus sealed tube	2761 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.077
Detector resolution: 9.091 pixels mm^{-1}	θ_{max} = 26.0º
T = 150(1) K	θ_{min} = 1.9º
φ and ω scans to fill the Ewald sphere	h = −17→17
Absorption correction: Gaussian integration (Coppens, 1970)	k = −18→18
T_{min} = 0.589, T_{max} = 0.672	l = −9→9
12191 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.041$	$w = 1/[\sigma^2(F_o^2) + (0.0365P)^2 + 0.6801P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.091$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.10$	$\Delta\rho_{max} = 0.34$ e Å^{-3}
3504 reflections	$\Delta\rho_{min} = -0.65$ e Å^{-3}
226 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), with how many Friedel pairs?
Secondary atom site location: difference Fourier map	Flack parameter: −0.005 (19)

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 $F^2 > 2\sigma(F^2)$ 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}
N6	0.2534 (3)	0.9161 (2)	0.9706 (4)	0.0416 (9)
Ni1	0.08457 (3)	0.76671 (3)	0.31260 (6)	0.02371 (13)
N30	0.21241 (19)	0.75188 (17)	0.1877 (4)	0.0340 (7)
H30A	0.2321	0.8043	0.1511	0.041*
H30B	0.2552	0.7305	0.2577	0.041*
N20	0.0409 (2)	0.8673 (2)	0.1579 (4)	0.0374 (9)
H20A	−0.0103	0.8924	0.2000	0.045*
H20B	0.0853	0.9083	0.1508	0.045*
N1	0.1272 (2)	0.6611 (2)	0.4640 (5)	0.0364 (9)
N4	0.1296 (2)	0.8525 (2)	0.4893 (4)	0.0325 (8)
N10	−0.0475 (2)	0.7439 (2)	0.4137 (4)	0.0412 (9)
H10A	−0.0420	0.7159	0.5111	0.049*
H10B	−0.0764	0.7951	0.4317	0.049*
C4	0.1484 (3)	0.9043 (2)	0.5869 (5)	0.0246 (8)
C5	0.1504 (2)	1.0555 (2)	0.6838 (6)	0.0278 (8)
N40	0.0362 (3)	0.6867 (2)	0.1225 (4)	0.0384 (9)
C6	0.2168 (3)	0.9393 (2)	0.8519 (5)	0.0292 (9)

N5	0.1342 (2)	1.1284 (2)	0.6661 (5)	0.0396 (8)
C1	0.1529 (3)	0.6058 (3)	0.5481 (6)	0.0288 (9)
C8	0.1717 (2)	0.9662 (2)	0.7062 (5)	0.0264 (8)
C3	0.2745 (3)	0.5457 (2)	0.7152 (5)	0.0312 (9)
C7	0.1853 (2)	0.5385 (2)	0.6483 (4)	0.0250 (9)
N2	0.0849 (3)	0.4021 (2)	0.6862 (6)	0.0684 (13)
C2	0.1307 (3)	0.4627 (3)	0.6701 (6)	0.0371 (10)
N3	0.3479 (3)	0.5551 (2)	0.7663 (5)	0.0498 (11)
C22	−0.0020 (3)	0.7412 (3)	−0.0137 (6)	0.0605 (14)
H22A	0.0209	0.7189	−0.1182	0.073*
H22B	−0.0689	0.7354	−0.0144	0.073*
C12	−0.0379 (3)	0.6326 (3)	0.1968 (7)	0.0486 (12)
H12A	−0.0106	0.5884	0.2676	0.058*
H12B	−0.0723	0.6031	0.1101	0.058*
C31	0.2008 (3)	0.6913 (3)	0.0461 (6)	0.0490 (12)
H31A	0.2556	0.6551	0.0354	0.059*
H31B	0.1938	0.7248	−0.0549	0.059*
C32	0.1169 (3)	0.6337 (3)	0.0701 (6)	0.0493 (13)
H32A	0.1026	0.6039	−0.0326	0.059*
H32B	0.1302	0.5898	0.1533	0.059*
C11	−0.1030 (3)	0.6896 (3)	0.2970 (7)	0.0506 (12)
H11A	−0.1384	0.7272	0.2239	0.061*
H11B	−0.1460	0.6532	0.3583	0.061*
C21	0.0215 (5)	0.8334 (4)	−0.0015 (7)	0.0778 (19)
H21A	0.0751	0.8439	−0.0709	0.093*
H21B	−0.0295	0.8668	−0.0477	0.093*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N6	0.054 (2)	0.044 (2)	0.027 (2)	0.0077 (18)	0.0011 (18)	0.0044 (17)
Ni1	0.0241 (2)	0.0228 (2)	0.0243 (2)	0.00161 (19)	−0.0009 (2)	−0.0035 (2)
N30	0.0366 (16)	0.0288 (19)	0.0366 (18)	0.0020 (12)	0.0076 (16)	0.0033 (18)
N20	0.0310 (17)	0.0383 (19)	0.043 (2)	0.0058 (15)	−0.0072 (16)	0.0025 (18)
N1	0.0317 (19)	0.033 (2)	0.044 (2)	−0.0041 (15)	0.0032 (17)	0.0078 (19)
N4	0.0374 (19)	0.0265 (19)	0.034 (2)	−0.0008 (15)	−0.0053 (16)	0.0011 (17)
N10	0.0303 (16)	0.040 (2)	0.054 (2)	−0.0032 (14)	0.0055 (16)	−0.0206 (18)
C4	0.026 (2)	0.025 (2)	0.023 (2)	0.0014 (15)	0.0001 (16)	0.0043 (18)
C5	0.0276 (18)	0.035 (2)	0.021 (2)	−0.0020 (15)	0.0008 (19)	−0.001 (2)
N40	0.045 (2)	0.038 (2)	0.032 (2)	0.0013 (16)	−0.0033 (16)	−0.0131 (16)
C6	0.033 (2)	0.027 (2)	0.027 (3)	0.0026 (16)	0.0073 (17)	−0.0027 (17)
N5	0.051 (2)	0.0295 (19)	0.038 (2)	0.0038 (16)	−0.0027 (18)	0.0054 (18)
C1	0.028 (2)	0.030 (2)	0.028 (2)	−0.0051 (17)	0.0049 (18)	−0.003 (2)
C8	0.037 (2)	0.0220 (19)	0.020 (2)	0.0016 (14)	−0.0013 (18)	0.0022 (18)
C3	0.044 (3)	0.028 (2)	0.022 (2)	−0.0044 (17)	0.007 (2)	0.0047 (18)
C7	0.033 (2)	0.0234 (19)	0.019 (2)	−0.0063 (15)	0.0000 (16)	0.0016 (16)
N2	0.086 (3)	0.055 (2)	0.064 (3)	−0.038 (2)	−0.035 (3)	0.031 (3)
C2	0.051 (2)	0.037 (2)	0.023 (2)	−0.0095 (19)	−0.016 (2)	0.011 (2)

N3	0.042 (2)	0.053 (2)	0.054 (3)	−0.0079 (18)	−0.0077 (18)	0.0130 (19)
C22	0.071 (3)	0.068 (4)	0.042 (3)	0.010 (3)	−0.024 (2)	−0.013 (3)
C12	0.044 (2)	0.039 (2)	0.062 (3)	−0.0110 (19)	0.000 (3)	−0.023 (3)
C31	0.058 (3)	0.047 (3)	0.042 (3)	0.009 (2)	0.022 (2)	−0.004 (2)
C32	0.070 (3)	0.041 (3)	0.037 (3)	0.004 (2)	0.011 (2)	−0.022 (2)
C11	0.028 (2)	0.052 (3)	0.072 (4)	−0.0100 (17)	0.005 (2)	−0.019 (3)
C21	0.109 (5)	0.068 (4)	0.057 (4)	−0.019 (3)	−0.052 (3)	0.018 (3)

Geometric parameters (Å, °)

Ni1—N4	2.045 (4)	N6—C6	1.152 (5)
Ni1—N20	2.080 (3)	C6—C8	1.408 (6)
Ni1—N40	2.085 (3)	C1—C7	1.391 (6)
Ni1—N10	2.104 (3)	C3—N3	1.146 (5)
Ni1—N30	2.116 (3)	C3—C7	1.401 (6)
Ni1—N1	2.118 (4)	C7—C2	1.413 (5)
N30—C31	1.482 (5)	N2—C2	1.145 (5)
N30—H30A	0.9000	C22—C21	1.453 (7)
N30—H30B	0.9000	C22—H22A	0.9700
N20—C21	1.418 (6)	C22—H22B	0.9700
N20—H20A	0.9000	C12—C11	1.517 (6)
N20—H20B	0.9000	C12—H12A	0.9700
N1—C1	1.146 (5)	C12—H12B	0.9700
N4—C4	1.151 (5)	C31—C32	1.509 (6)
N10—C11	1.490 (5)	C31—H31A	0.9700
N10—H10A	0.9000	C31—H31B	0.9700
N10—H10B	0.9000	C32—H32A	0.9700
C4—C8	1.393 (6)	C32—H32B	0.9700
C5—N5	1.148 (4)	C11—H11A	0.9700
C5—C8	1.411 (5)	C11—H11B	0.9700
N40—C12	1.479 (6)	C21—H21A	0.9700
N40—C32	1.482 (5)	C21—H21B	0.9700
N40—C22	1.488 (6)		
N4—Ni1—N20	92.46 (14)	C4—C8—C6	119.5 (3)
N4—Ni1—N40	176.02 (14)	C4—C8—C5	121.1 (4)
N20—Ni1—N40	83.56 (14)	C6—C8—C5	119.4 (4)
N4—Ni1—N10	97.05 (13)	N3—C3—C7	176.9 (4)
N20—Ni1—N10	94.67 (14)	C1—C7—C3	118.4 (3)
N40—Ni1—N10	83.42 (14)	C1—C7—C2	119.5 (3)
N4—Ni1—N30	97.20 (13)	C3—C7—C2	122.0 (3)
N20—Ni1—N30	93.24 (13)	N2—C2—C7	178.6 (5)
N40—Ni1—N30	82.96 (13)	C21—C22—N40	114.0 (4)
N10—Ni1—N30	163.37 (12)	C21—C22—H22A	108.8
N4—Ni1—N1	89.55 (13)	N40—C22—H22A	108.8
N20—Ni1—N1	177.99 (14)	C21—C22—H22B	108.8
N40—Ni1—N1	94.43 (14)	N40—C22—H22B	108.8
N10—Ni1—N1	84.97 (14)	H22A—C22—H22B	107.7
N30—Ni1—N1	86.61 (12)	N40—C12—C11	110.1 (3)
C31—N30—Ni1	109.7 (2)	N40—C12—H12A	109.6

C31—N30—H30A	109.7	C11—C12—H12A	109.6
Ni1—N30—H30A	109.7	N40—C12—H12B	109.6
C31—N30—H30B	109.7	C11—C12—H12B	109.6
Ni1—N30—H30B	109.7	H12A—C12—H12B	108.2
H30A—N30—H30B	108.2	N30—C31—C32	110.9 (4)
C21—N20—Ni1	109.7 (3)	N30—C31—H31A	109.5
C21—N20—H20A	109.7	C32—C31—H31A	109.5
Ni1—N20—H20A	109.7	N30—C31—H31B	109.5
C21—N20—H20B	109.7	C32—C31—H31B	109.5
Ni1—N20—H20B	109.7	H31A—C31—H31B	108.1
H20A—N20—H20B	108.2	N40—C32—C31	110.4 (4)
C1—N1—Ni1	177.5 (3)	N40—C32—H32A	109.6
C4—N4—Ni1	174.6 (3)	C31—C32—H32A	109.6
C11—N10—Ni1	109.5 (2)	N40—C32—H32B	109.6
C11—N10—H10A	109.8	C31—C32—H32B	109.6
Ni1—N10—H10A	109.8	H32A—C32—H32B	108.1
C11—N10—H10B	109.8	N10—C11—C12	109.0 (3)
Ni1—N10—H10B	109.8	N10—C11—H11A	109.9
H10A—N10—H10B	108.2	C12—C11—H11A	109.9
N4—C4—C8	179.4 (4)	N10—C11—H11B	109.9
N5—C5—C8	179.1 (4)	C12—C11—H11B	109.9
C12—N40—C32	112.3 (3)	H11A—C11—H11B	108.3
C12—N40—C22	110.3 (4)	N20—C21—C22	117.5 (4)
C32—N40—C22	112.7 (4)	N20—C21—H21A	107.9
C12—N40—Ni1	105.7 (3)	C22—C21—H21A	107.9
C32—N40—Ni1	105.5 (3)	N20—C21—H21B	107.9
C22—N40—Ni1	110.0 (3)	C22—C21—H21B	107.9
N6—C6—C8	179.0 (4)	H21A—C21—H21B	107.2
N1—C1—C7	179.1 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N30—H30A···N6^{i}	0.90	2.27	3.119 (5)	158
N30—H30B···N5^{ii}	0.90	2.32	3.141 (4)	152
N20—H20A···N3^{iii}	0.90	2.22	3.090 (5)	164
N20—H20B···N3^{iv}	0.90	2.53	3.347 (5)	151
N10—H10A···N2^{v}	0.90	2.38	3.183 (6)	149
N10—H10B···N5^{vi}	0.90	2.38	3.090 (5)	136

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) −*x*+1/2, *y*−1/2, −*z*+1; (iii) *x*−1/2, −*y*+3/2, −*z*+1; (iv) −*x*+1/2, *y*+1/2, −*z*+1; (v) −*x*, −*y*+1, *z*; (vi) −*x*, −*y*+2, *z*.

Fig. 1

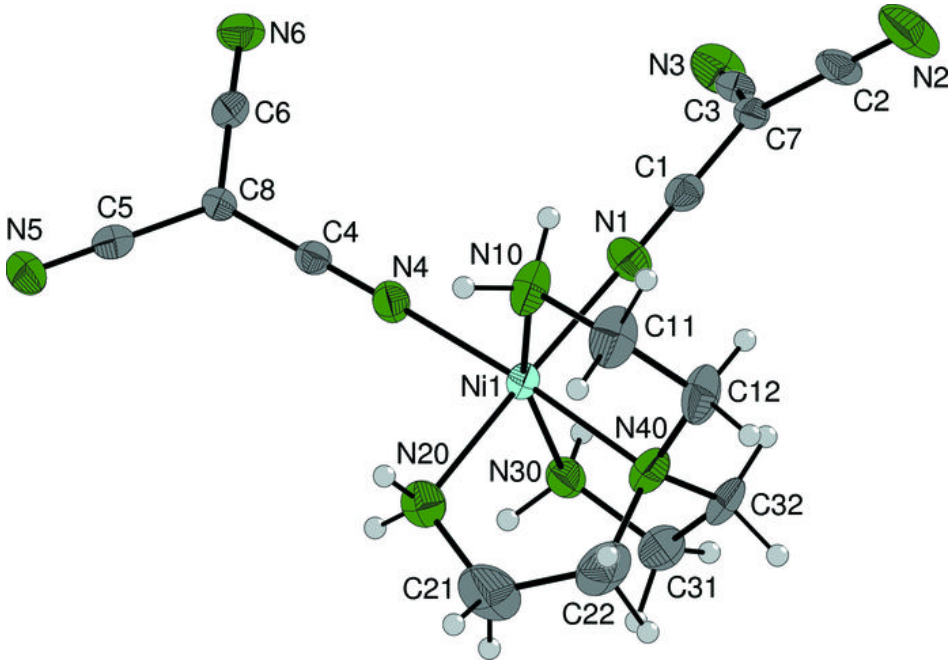

N6
C6
C8
C5
N5
C4
N4
N10
N1
C1
N3
C3
C7
C2
N2
C11
Ni1
C12
N40
N20
N30
C32
C21
C22
C31

Fig. 2