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Di-μ-azido-κ^4N:N-bis[(azido-κN)(2,9-dimethyl-1,10-phenanthroline-κ^2N,N')-nickel(II)]

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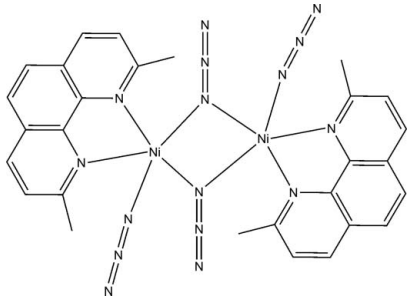
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.004 Å; R factor = 0.033; wR factor = 0.083; data-to-parameter ratio = 16.2.

The title complex, $[Ni_2(N_3)_4(C_{14}H_{12}N_2)_2]$, is a centrosymmetric dimer in which each Ni^{II} atom is coordinated by five N atoms (two from a 2,9-dimethyl-1,10-phenanthroline ligand, two from the bridging azide group and one from the terminal azide) in a slightly distorted square-pyramidal geometry. The Ni···Ni distance is 3.2532 (9) Å. In the crystal structure, molecules are linked into one-dimensional chains by C—H···N hydrogen bonds and π–π stacking interactions [π-π interaction distance = 3.6215 (16) Å].

Related literature

For related literature, see: Cai *et al.* (2007); Grove *et al.* (2001); Li *et al.* (2005); Qian *et al.* (2007); Wang *et al.* (2004); You (2005); Zhao *et al.* (2003).



Experimental

Crystal data

$[Ni_2(N_3)_4(C_{14}H_{12}N_2)_2]$
M_r = 702.01
Monoclinic, $C2/c$
a = 13.471 (3) Å
b = 11.226 (2) Å
c = 19.605 (4) Å
β = 94.36 (3)°
V = 2956.2 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.33 mm^{-1}
T = 153 (2) K
0.10 × 0.10 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.879, T_{max} = 0.937
6614 measured reflections
3396 independent reflections
1923 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.083
S = 0.93
3396 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14A···N3^{i}	0.96	2.47	3.391 (4)	162
C4—H4···N8^{ii}	0.93	2.43	3.304 (4)	157

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *maXus* (Mackay *et al.*, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: PK2037).

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supplementary materials

Acta Cryst. (2007). E**63**, m2211 [**doi:10.1107/S1600536807035313**]

Di-μ-azido-κ^4N:*N*-bis[(azido-κN)(2,9-dimethyl-1,10-phenanthroline-κ^2N,*N*')nickel(II)]

L.-L. Li and T.-F. Liu

Comment

The azide ion is a versatile ligand, it can bind metal ions in a number of coordination modes, giving rise to mononuclear, dinuclear and polynuclear complexes. In these complexes different types of bonding of the azido ligands have been observed; either simple monodentate terminal fashion or bridging end-to-end (1,3-di-μ) or end-on (1,1-di-μ) modes (Grove *et al.*, 2001; Zhao *et al.*, 2003; Wang *et al.*, 2004; Li *et al.*, 2005; You, 2005; Qian *et al.*, 2007; Cai *et al.*, 2007).

The title compound is centrosymmetric. In this complex, the two nickel(II) atoms are doubly bridged by two end-on azido groups (Fig 1). Each nickel atom is located in a slightly distored square-pyramidal geometry, being surrounded by five nitrogen atoms (two of a 2,9-dimethyl-1,10-phenanthroline, two of the bridging azido group and the last one of the terminal azide). A N atom of the 2,9-dimethyl-1,10-phenanthroline is located in the axial position and the ligand bond lengths and angles fall in the ranges of 1.985 (2)–2.070 (2) Å and 76.09 (9)–160.44 (9)°, respectively. The Ni···Ni distance is 3.2532 (9) Å.

π–π interactions between the phenanthroline rings (Fig. 2) is observed with a *Cg*(6)-*Cg*(6)^{i} (ring *Cg*(6): C5, C6, C7, C8, C12, C13; symmetry code: (i) $-x$, y, 1/2 − z) distance of 3.6215 (16) Å. These π-π stacking interactions and C—H···N hydrogen bonds lead to one dimensional chains.

Experimental

The title compound was sythesized as follows: To a methanolic solution (10 ml) of nickel(II) perchlorate hexahydrate (0.183 g, 0.5 mmol), 2,9-dimethyl-1,10-phenanthroline (0.104 g, 0.5 mmol) and sodium azide (0.046 g, 0.7 mmol) were added with stirring. The resulting green solution was stirred for 0.5 h at room temperature. Slow evaporation of the solution yielded a green crystalline compound.

Refinement

The hydrogen atoms were assigned with isotropic displacement factors and included in the final refinement cycles by use of geometrical restraints (C_{ar}–H = 0.93 Å; C_{Me}–H = 0.96 Å).

Figures

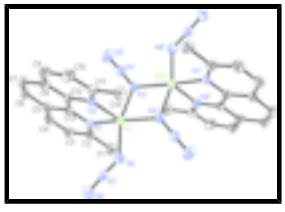

Fig. 1. The title compound, showing 30% probability displacement ellipsoids (Symmetry codes: $-x$ + 3/2, $-y$ + 3/2, $-z$ + 2). Hydrogen atoms are omitted for clarity.

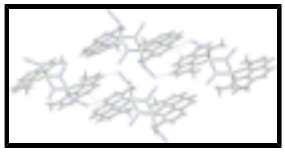

Fig. 2. The intermolecular π-π stacking and C—H···N interactions.

Di-μ-azido-κ^4*N*:*N*-bis[(azido-κ*N*)(2,9-dimethyl-1,10-phenanthroline- κ*N*,*N*)nickel(II)]

Crystal data

$[Ni_2(N_3)_4(C_{14}H_{12}N_2)_2]$	F_{000} = 1440
M_r = 702.01	D_x = 1.577 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 13380 reflections
a = 13.471 (3) Å	θ = 3.4–27.5º
b = 11.226 (2) Å	μ = 1.33 mm^{-1}
c = 19.605 (4) Å	*T* = 153 (2) K
β = 94.36 (3)º	Block, green
V = 2956.2 (10) Å^3	0.10 × 0.10 × 0.05 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	3396 independent reflections
Radiation source: fine-focus sealed tube	1923 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.032
Detector resolution: 18 pixels mm^{-1}	θ_{max} = 27.5º
T = 153(2) K	θ_{min} = 3.6º
ω scans	*h* = −17→17
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*k* = −14→14
T_{min} = 0.879, T_{max} = 0.937	*l* = −25→25
6614 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.033	H-atom parameters constrained
$wR(F^2)$ = 0.083	$w = 1/[\sigma^2(F_o^2) + (0.0402P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.93	$(\Delta/\sigma)_{max}$ = 0.002
3396 reflections	$\Delta\rho_{max}$ = 0.31 e Å^{-3}
210 parameters	$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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}
Ni1	0.84958 (2)	0.75286 (3)	0.958017 (13)	0.03719 (11)
N1	0.86582 (14)	0.8208 (2)	0.86198 (10)	0.0385 (5)
C12	0.86702 (16)	0.6124 (2)	0.83785 (12)	0.0385 (6)
N2	0.86412 (14)	0.59478 (19)	0.90696 (10)	0.0387 (5)
C13	0.86592 (17)	0.7327 (2)	0.81366 (12)	0.0378 (6)
N3	0.69573 (14)	0.7560 (2)	0.94405 (9)	0.0436 (5)
N4	0.64685 (16)	0.7357 (2)	0.89104 (11)	0.0483 (6)
C7	0.8734 (2)	0.5456 (3)	0.71970 (13)	0.0568 (8)
H7	0.8757	0.4837	0.6884	0.068*
N7	1.05529 (18)	0.8271 (2)	0.96773 (10)	0.0521 (6)
C3	0.8736 (2)	0.9632 (3)	0.77282 (14)	0.0535 (8)
H3	0.8767	1.0427	0.7600	0.064*
C2	0.87088 (18)	0.9336 (2)	0.84214 (13)	0.0430 (6)
C5	0.86905 (18)	0.7572 (3)	0.74372 (12)	0.0447 (6)
C9	0.8781 (2)	0.4033 (3)	0.81853 (15)	0.0578 (8)
H9	0.8826	0.3379	0.7898	0.069*
N6	0.98706 (17)	0.7894 (2)	0.99584 (11)	0.0542 (6)
C4	0.8717 (2)	0.8767 (3)	0.72427 (13)	0.0526 (7)
H4	0.8721	0.8971	0.6783	0.063*
C8	0.87256 (19)	0.5188 (3)	0.79084 (14)	0.0480 (7)
C11	0.86797 (19)	0.4847 (2)	0.93092 (13)	0.0441 (6)
C14	0.8643 (2)	0.4653 (3)	1.00651 (13)	0.0579 (8)
H14A	0.8584	0.5408	1.0289	0.087*
H14B	0.9243	0.4263	1.0242	0.087*
H14C	0.8079	0.4165	1.0147	0.087*
C10	0.8768 (2)	0.3867 (3)	0.88718 (15)	0.0574 (8)
H10	0.8818	0.3101	0.9053	0.069*
C6	0.8709 (2)	0.6584 (3)	0.69726 (13)	0.0554 (8)
H6	0.8703	0.6731	0.6505	0.066*
C1	0.8750 (2)	1.0281 (2)	0.89582 (14)	0.0564 (8)
H1A	0.8671	0.9925	0.9396	0.085*

H1B	0.8225	1.0846	0.8855	0.085*
H1C	0.9381	1.0681	0.8969	0.085*
N5	0.6021 (2)	0.7173 (3)	0.84052 (13)	0.0829 (10)
N8	1.1259 (2)	0.8620 (3)	0.94390 (13)	0.0916 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.03987 (17)	0.04148 (19)	0.03020 (15)	0.00079 (17)	0.00262 (12)	−0.00298 (16)
N1	0.0378 (12)	0.0427 (14)	0.0352 (11)	−0.0019 (10)	0.0031 (9)	−0.0022 (10)
C12	0.0307 (13)	0.0469 (16)	0.0379 (13)	0.0008 (12)	0.0026 (11)	−0.0072 (12)
N2	0.0375 (11)	0.0405 (13)	0.0378 (11)	0.0007 (9)	0.0016 (9)	−0.0017 (10)
C13	0.0315 (11)	0.0489 (18)	0.0331 (11)	−0.0004 (12)	0.0036 (10)	−0.0063 (11)
N3	0.0400 (11)	0.0604 (14)	0.0301 (10)	0.0029 (12)	0.0007 (8)	−0.0045 (11)
N4	0.0450 (12)	0.0616 (16)	0.0387 (12)	0.0033 (12)	0.0056 (10)	−0.0013 (12)
C7	0.0546 (18)	0.074 (2)	0.0422 (17)	−0.0017 (17)	0.0045 (13)	−0.0214 (15)
N7	0.0510 (14)	0.0706 (17)	0.0339 (11)	−0.0038 (13)	−0.0015 (10)	−0.0121 (11)
C3	0.0541 (18)	0.054 (2)	0.0530 (18)	−0.0014 (14)	0.0056 (14)	0.0106 (14)
C2	0.0415 (15)	0.0453 (17)	0.0422 (15)	−0.0016 (12)	0.0021 (12)	0.0022 (12)
C5	0.0364 (12)	0.0635 (17)	0.0340 (12)	−0.0007 (15)	0.0022 (10)	−0.0026 (15)
C9	0.0597 (18)	0.051 (2)	0.0619 (19)	0.0039 (15)	−0.0001 (15)	−0.0226 (15)
N6	0.0458 (13)	0.0739 (17)	0.0424 (12)	−0.0062 (12)	−0.0006 (10)	0.0011 (11)
C4	0.0489 (17)	0.073 (2)	0.0363 (14)	0.0010 (16)	0.0068 (12)	0.0094 (14)
C8	0.0405 (16)	0.0505 (19)	0.0529 (16)	−0.0006 (13)	0.0031 (13)	−0.0147 (14)
C11	0.0421 (15)	0.0406 (16)	0.0490 (15)	0.0017 (12)	0.0008 (12)	−0.0010 (13)
C14	0.070 (2)	0.0483 (18)	0.0554 (17)	0.0037 (15)	0.0061 (15)	0.0074 (14)
C10	0.067 (2)	0.0369 (17)	0.0672 (19)	0.0041 (14)	−0.0007 (16)	−0.0053 (14)
C6	0.0545 (18)	0.078 (2)	0.0335 (14)	−0.0002 (16)	0.0052 (13)	−0.0108 (15)
C1	0.073 (2)	0.0430 (19)	0.0530 (17)	−0.0016 (15)	0.0015 (15)	−0.0015 (14)
N5	0.078 (2)	0.123 (3)	0.0460 (15)	−0.0035 (17)	−0.0102 (13)	−0.0129 (16)
N8	0.077 (2)	0.145 (3)	0.0561 (16)	−0.042 (2)	0.0206 (15)	−0.0117 (18)

Geometric parameters (Å, °)

Ni1—N6	1.985 (2)	C3—C4	1.358 (4)
Ni1—N2	2.054 (2)	C3—C2	1.402 (3)
Ni1—N1	2.058 (2)	C3—H3	0.9300
Ni1—N3^{i}	2.0607 (19)	C2—C1	1.492 (4)
Ni1—N3	2.070 (2)	C5—C4	1.396 (4)
N1—C2	1.329 (3)	C5—C6	1.436 (4)
N1—C13	1.369 (3)	C9—C10	1.360 (4)
C12—N2	1.373 (3)	C9—C8	1.405 (4)
C12—C8	1.404 (3)	C9—H9	0.9300
C12—C13	1.431 (4)	C4—H4	0.9300
N2—C11	1.322 (3)	C11—C10	1.405 (4)
C13—C5	1.402 (3)	C11—C14	1.502 (3)
N3—N4	1.209 (3)	C14—H14A	0.9600
N3—Ni1^{i}	2.0607 (19)	C14—H14B	0.9600

N4—N5	1.138 (3)	C14—H14C	0.9600
C7—C6	1.340 (4)	C10—H10	0.9300
C7—C8	1.428 (4)	C6—H6	0.9300
C7—H7	0.9300	C1—H1A	0.9600
N7—N8	1.159 (3)	C1—H1B	0.9600
N7—N6	1.185 (3)	C1—H1C	0.9600
N6—Ni1—N2	103.88 (9)	C3—C2—C1	120.9 (3)
N6—Ni1—N1	95.98 (9)	C4—C5—C13	117.3 (2)
N2—Ni1—N1	81.58 (8)	C4—C5—C6	124.5 (2)
N6—Ni1—N3^{i}	89.76 (9)	C13—C5—C6	118.2 (3)
N2—Ni1—N3^{i}	117.29 (8)	C10—C9—C8	120.3 (3)
N1—Ni1—N3^{i}	158.38 (9)	C10—C9—H9	119.9
N6—Ni1—N3	160.44 (9)	C8—C9—H9	119.9
N2—Ni1—N3	94.69 (8)	N7—N6—Ni1	129.40 (19)
N1—Ni1—N3	92.73 (8)	C3—C4—C5	119.7 (2)
N3^{i}—Ni1—N3	76.09 (9)	C3—C4—H4	120.2
C2—N1—C13	118.9 (2)	C5—C4—H4	120.2
C2—N1—Ni1	129.23 (17)	C12—C8—C9	116.2 (3)
C13—N1—Ni1	111.79 (17)	C12—C8—C7	119.2 (3)
N2—C12—C8	123.2 (3)	C9—C8—C7	124.6 (3)
N2—C12—C13	117.6 (2)	N2—C11—C10	121.2 (2)
C8—C12—C13	119.3 (2)	N2—C11—C14	118.9 (2)
C11—N2—C12	118.8 (2)	C10—C11—C14	120.0 (2)
C11—N2—Ni1	129.58 (17)	C11—C14—H14A	109.5
C12—N2—Ni1	111.56 (16)	C11—C14—H14B	109.5
N1—C13—C5	122.5 (2)	H14A—C14—H14B	109.5
N1—C13—C12	116.9 (2)	C11—C14—H14C	109.5
C5—C13—C12	120.6 (2)	H14A—C14—H14C	109.5
N4—N3—Ni1^{i}	127.69 (16)	H14B—C14—H14C	109.5
N4—N3—Ni1	125.79 (15)	C9—C10—C11	120.3 (3)
Ni1^{i}—N3—Ni1	103.91 (9)	C9—C10—H10	119.9
N5—N4—N3	178.8 (3)	C11—C10—H10	119.9
C6—C7—C8	121.2 (3)	C7—C6—C5	121.5 (3)
C6—C7—H7	119.4	C7—C6—H6	119.3
C8—C7—H7	119.4	C5—C6—H6	119.3
N8—N7—N6	175.6 (3)	C2—C1—H1A	109.5
C4—C3—C2	120.7 (3)	C2—C1—H1B	109.5
C4—C3—H3	119.7	H1A—C1—H1B	109.5
C2—C3—H3	119.7	C2—C1—H1C	109.5
N1—C2—C3	121.0 (2)	H1A—C1—H1C	109.5
N1—C2—C1	118.1 (2)	H1B—C1—H1C	109.5
N6—Ni1—N1—C2	−73.3 (2)	C13—N1—C2—C3	1.7 (4)
N2—Ni1—N1—C2	−176.5 (2)	Ni1—N1—C2—C3	−174.51 (18)
N3^{i}—Ni1—N1—C2	31.3 (4)	C13—N1—C2—C1	−177.5 (2)
N3—Ni1—N1—C2	89.1 (2)	Ni1—N1—C2—C1	6.3 (3)
N6—Ni1—N1—C13	110.21 (17)	C4—C3—C2—N1	−0.4 (4)
N2—Ni1—N1—C13	7.01 (15)	C4—C3—C2—C1	178.8 (3)

N3^{i}—Ni1—N1—C13	−145.1 (2)	N1—C13—C5—C4	−0.3 (3)
N3—Ni1—N1—C13	−87.32 (16)	C12—C13—C5—C4	−177.6 (2)
C8—C12—N2—C11	0.9 (3)	N1—C13—C5—C6	178.8 (2)
C13—C12—N2—C11	−178.1 (2)	C12—C13—C5—C6	1.5 (3)
C8—C12—N2—Ni1	−177.34 (18)	N2—Ni1—N6—N7	76.4 (3)
C13—C12—N2—Ni1	3.7 (3)	N1—Ni1—N6—N7	−6.4 (3)
N6—Ni1—N2—C11	82.1 (2)	N3^{i}—Ni1—N6—N7	−165.5 (3)
N1—Ni1—N2—C11	176.2 (2)	N3—Ni1—N6—N7	−122.4 (3)
N3^{i}—Ni1—N2—C11	−14.9 (2)	C2—C3—C4—C5	−1.3 (4)
N3—Ni1—N2—C11	−91.7 (2)	C13—C5—C4—C3	1.6 (4)
N6—Ni1—N2—C12	−99.89 (16)	C6—C5—C4—C3	−177.4 (3)
N1—Ni1—N2—C12	−5.77 (15)	N2—C12—C8—C9	−1.8 (4)
N3^{i}—Ni1—N2—C12	163.06 (14)	C13—C12—C8—C9	177.1 (2)
N3—Ni1—N2—C12	86.31 (16)	N2—C12—C8—C7	178.9 (2)
C2—N1—C13—C5	−1.4 (3)	C13—C12—C8—C7	−2.2 (4)
Ni1—N1—C13—C5	175.47 (17)	C10—C9—C8—C12	0.7 (4)
C2—N1—C13—C12	176.0 (2)	C10—C9—C8—C7	179.9 (3)
Ni1—N1—C13—C12	−7.2 (3)	C6—C7—C8—C12	1.3 (4)
N2—C12—C13—N1	2.4 (3)	C6—C7—C8—C9	−178.0 (3)
C8—C12—C13—N1	−176.6 (2)	C12—N2—C11—C10	1.2 (4)
N2—C12—C13—C5	179.8 (2)	Ni1—N2—C11—C10	179.08 (19)
C8—C12—C13—C5	0.8 (3)	C12—N2—C11—C14	−179.7 (2)
N6—Ni1—N3—N4	152.5 (3)	Ni1—N2—C11—C14	−1.8 (4)
N2—Ni1—N3—N4	−45.8 (2)	C8—C9—C10—C11	1.3 (4)
N1—Ni1—N3—N4	36.0 (2)	N2—C11—C10—C9	−2.3 (4)
N3^{i}—Ni1—N3—N4	−162.8 (3)	C14—C11—C10—C9	178.6 (3)
N6—Ni1—N3—Ni1^{i}	−44.8 (3)	C8—C7—C6—C5	1.1 (4)
N2—Ni1—N3—Ni1^{i}	116.97 (10)	C4—C5—C6—C7	176.5 (3)
N1—Ni1—N3—Ni1^{i}	−161.26 (10)	C13—C5—C6—C7	−2.5 (4)
N3^{i}—Ni1—N3—Ni1^{i}	0.0		

Symmetry codes: (i) −*x*+3/2, −*y*+3/2, −*z*+2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14A···N3^{i}	0.96	2.47	3.391 (4)	162
C4—H4···N8^{ii}	0.93	2.43	3.304 (4)	157

Symmetry codes: (i) −*x*+3/2, −*y*+3/2, −*z*+2; (ii) −*x*+2, *y*, −*z*+3/2.

Fig. 1

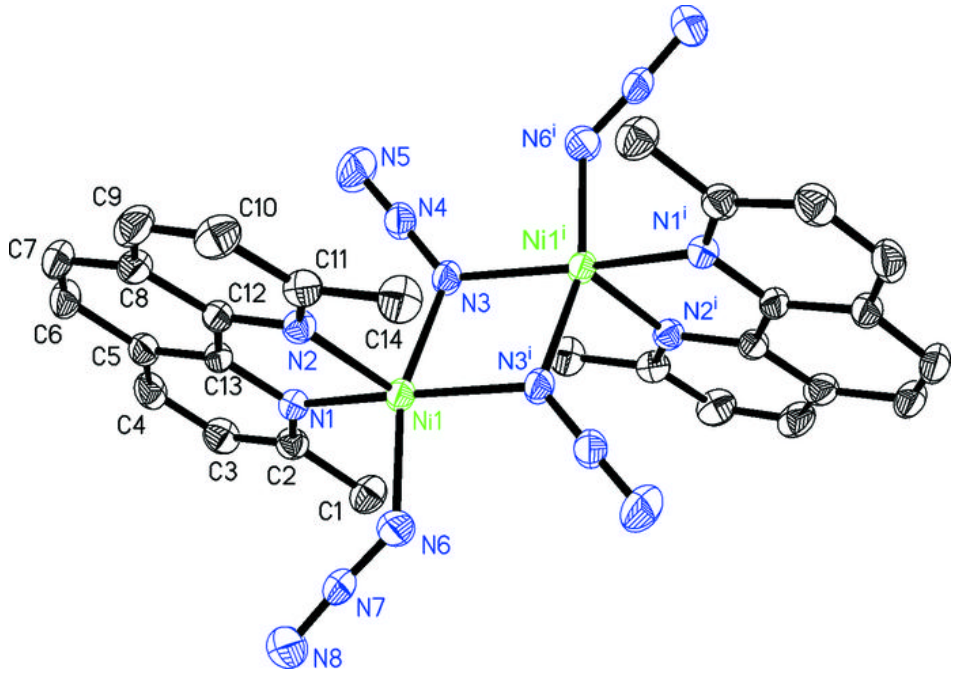
N6i
N5
N4
Ni1i
N1i
C9
C10
C7
C11
C8
C12
N3
N2i
C6
C14
N2
N3i
C5
C13
N1
Ni1
C4
C3
C2
C1
N6
N7
N8

Fig. 2