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Diazidodipyridinenickel(II)

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Key indicators

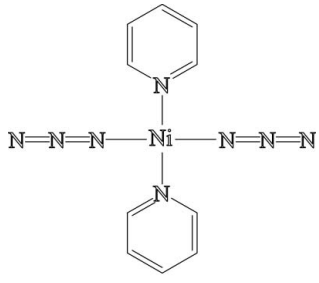
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.105
Data-to-parameter ratio = 14.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $[Ni(N_3)_2(C_5H_5N)_2]$, has two half-molecules in the asymmetric unit. One complete molecule is generated by twofold symmetry, the other by inversion. In this mononuclear compound, each Ni^{II} atom is coordinated by four N atoms from two pyridine molecules and two azide anions, thereby forming a slightly distorted square planar configuration.

Comment

In recent years, there has been considerable interest in the development of rational synthetic routes to coordination polymers by self-assembly (Munakata *et al.*, 1999). The prime strategy for designing these materials is to use a suitable bridging ligand (Koner *et al.*, 2003). Much attention has been paid to the azide anion and several azide-bridged complexes have been reported (Zhu *et al.*, 1999; You, 2005). Now, a new mononuclear azide-containing nickel complex, (I), is reported. There are two half-molecules in the asymmetric unit: the complete molecules are generated by twofold symmetry (Ni1, the rotation axis passing also through the pyridine N and *para*-C atoms) and by inversion (Ni2) (Fig. 1).



(I)

Both the Ni^{II} atoms are in a square-planar geometry, being coordinated by four N atoms from two *trans* pyridine molecules and two azide ions. The Ni—N bond lengths are normal (Table 1) and the *cis* and *trans* N—Ni—N angles show little deviation from ideal values. The dihedral angle between the N1- and N2-pyridine rings in the Ni1 molecule is 40.2 (3)°. The pyridine rings in the other molecule are exactly parallel by symmetry.

In the crystal structure of (I), the molecules interact with each other *via* weak C—H···N interactions, forming an extended network along the *a* axis (Fig. 2 and Table 2).

Experimental

Benzoic acid (1 mmol, 122 mg) and $Ni(NO_3)_2{\cdot}6H_2O$ (1 mmol, 290 mg) were suspended in a mixed solvent of pyridine and methanol

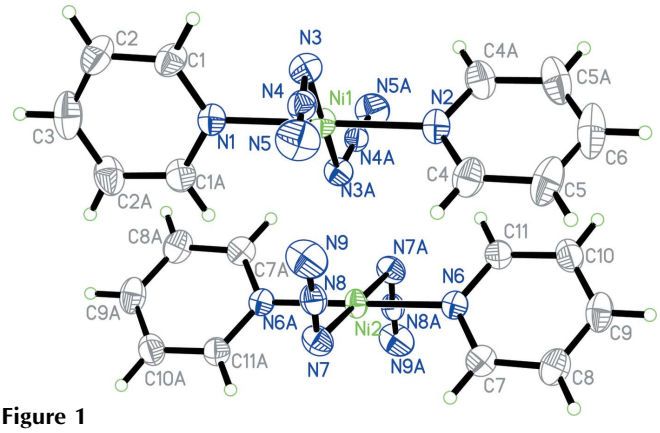


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms). [Symmetry codes: (A) $1-x, y, \frac{3}{2}-z$ for the upper molecule; $\frac{1}{2}-x, \frac{1}{2}-y, 1-z$ for the lower molecule.]

(1:1 *v*/*v*, 10 ml). To this solution was added an aqueous solution (2 ml) of NaN_3 (1 mmol, 65 mg). The resulting solution was stirred for 20 min and then filtered. After keeping the filtrate in air for 15 d, large blue block-shaped crystals of (I) formed at the bottom of the vessel. The crystals were isolated, washed three times with water and dried in a vacuum desiccator over $CaCl_2$ (yield 84.6%). Analysis found: C 39.55, H 3.25, N 37.80%; calculated for $C_{10}H_{10}NiN_8$: C 39.91, H 3.35, N 37.24%.

Crystal data

$[Ni(N_3)_2(C_5H_5N)_2]$
$M_r = 300.95$
Monoclinic, $C2/c$
$a = 12.7646\ (16)$ Å
$b = 14.1998\ (16)$ Å
$c = 14.1347\ (17)$ Å
$\beta = 100.766\ (3)^\circ$
$V = 2516.9\ (5)$ Å^3
$Z = 8$
$D_x = 1.588$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.54$ mm^{-1}
$T = 293\ (2)$ K
Block, blue
0.35 × 0.31 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.589$, $T_{max} = 0.735$
6765 measured reflections
2593 independent reflections
2061 reflections with $I > 2\sigma(I)$
$R_{int} = 0.070$
$\theta_{max} = 26.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.105$
$S = 1.04$
2593 reflections
176 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 0.0859P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.48$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—N3	2.000 (2)	Ni2—N7	2.003 (2)
Ni1—N1	2.057 (3)	Ni2—N6	2.017 (2)
Ni1—N2	2.073 (3)		

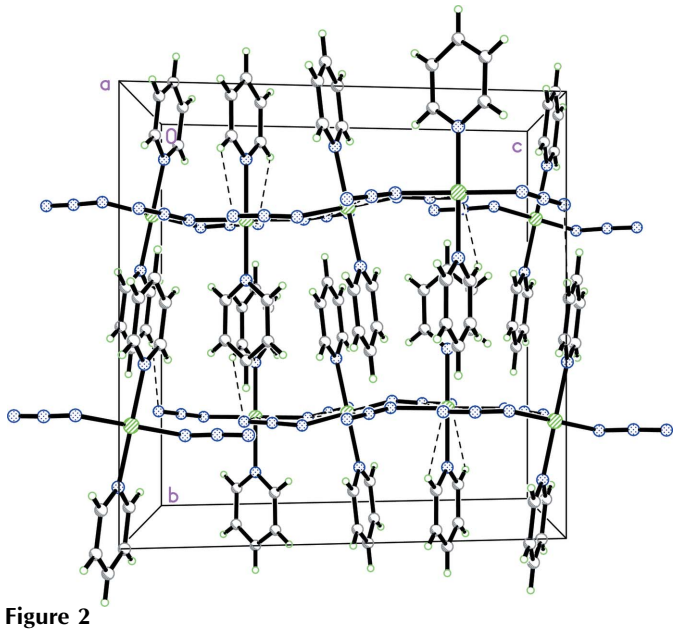


Figure 2
The crystal packing of (I), viewed along the *a* axis, with C—H···N interactions shown as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···N9^{i}	0.93	2.49	3.182 (5)	131

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

H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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