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Diazidotetraimidazolenickel(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.032
wR factor = 0.092
Data-to-parameter ratio = 13.0

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

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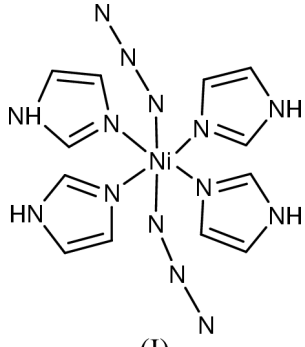
In the title complex, $[Ni(N_3)_2(C_3H_4N_2)_4]$, the octahedrally coordinated Ni atom, which is located at an inversion center, is coordinated by four N atoms of imidazole and two N atoms of azide ligands. The molecules are linked into a three-dimensional network through N—H···N hydrogen bonds.

Comment

Nickel(II)–azido systems have been widely studied from structural and magnetic points of view in recent years. The azide ligand can act not only as a highly effective super-exchange pathway, giving antiferromagnetic coupling for end-to-end coordination between two nickel ions or ferromagnetic coupling for end-on coordination, but can also generate different nuclearity compounds (Arriortua *et al.*, 1990; Cortes *et al.*, 1992; Vicente *et al.*, 1993, 1995; Ribas *et al.*, 1993; Escuer *et al.*, 1995, 1996). On the other hand, nickel(II)–imidazole interactions are important in biological processes. We report here the synthesis and crystal structure of a new compound, (I), simultaneously containing imidazole and azide ligands.



(I)

As shown in Fig. 1, the Ni atom is located at the inversion center of the molecule, and is coordinated by four imidazole ligands and two azide ligands. The Ni1—N7 and Ni1—N5 bond distances are 2.095 (2) and 2.124 (2) Å, respectively (Table 1). The Ni1—N3 bond distance is 2.131 (2) Å, which is longer than that found in other nickel–azide compounds [1.991 (5) (Escuer *et al.*, 1996), 1.872 (5) (Becalska *et al.*, 1992) and 2.018 (8) Å (Enemark, 1971)]. The complex forms a three-dimensional network through N—H···N intermolecular hydrogen bonds (Fig. 2 and Table 2).

Experimental

To a methanol–acetone solution (1:1, 20 ml) of nickel chloride (1.00 g, 4.2 mmol) were added imidazole (1.00 g, 14.7 mmol) and sodium azide (0.60 g, 9.2 mmol). The mixture was refluxed for 30 min, then allowed to cool to room temperature. Blue prism-shaped crystals of (I) suitable for X-ray analysis were obtained after a few days.

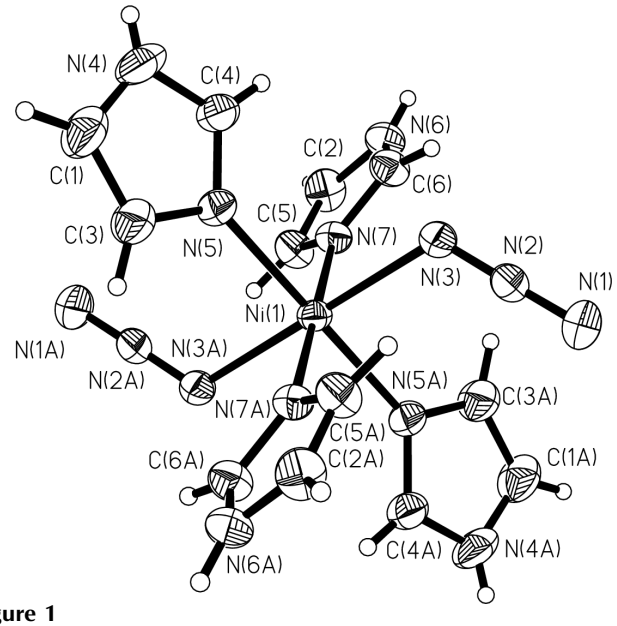


Figure 1
A perspective view of the complete centrosymmetric molecule of (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (*A*) $-x, 1-y, 1-z$.]

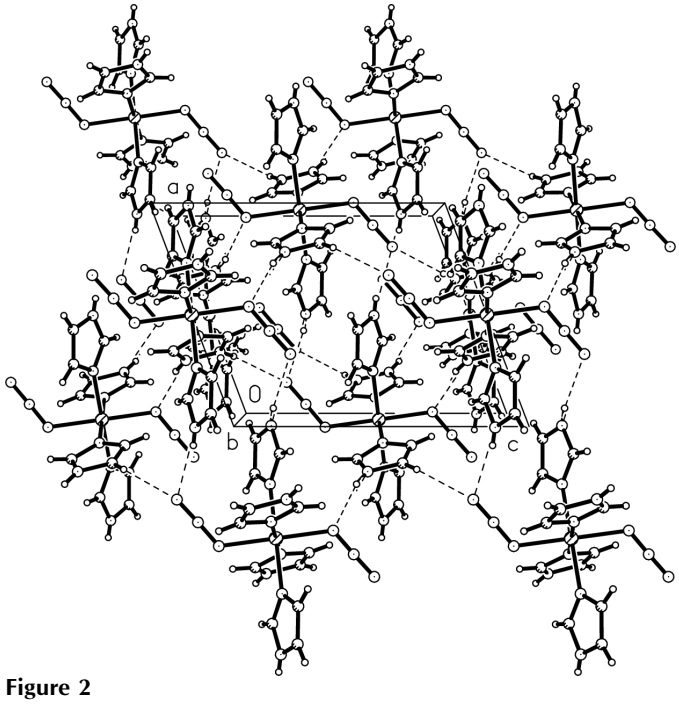


Figure 2
Cell packing diagram of (I), viewed along the *b* axis. Hydrogen bonds are indicated by dashed lines.

Crystal data

$[Ni(N_3)_2(C_3H_4N_2)_4]$
$M_r = 415.10$
Monoclinic, $P2_1/n$
$a = 8.787\ (1)$ Å
$b = 10.464\ (1)$ Å
$c = 10.866\ (1)$ Å
$\beta = 110.67\ (1)^\circ$
$V = 934.79\ (17)$ Å^3
$Z = 2$
$D_x = 1.475$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2860 reflections
$\theta = 2.0$–25.0°
$\mu = 1.07$ mm^{-1}
$T = 293\ (2)$ K
Prism, blue
$0.32 \times 0.23 \times 0.16$ mm

Data collection

Siemens SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.706$, $T_{max} = 0.843$
2860 measured reflections
1630 independent reflections
1340 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 25.0^\circ$
$h = -10 \rightarrow 8$
$k = -12 \rightarrow 8$
$l = -6 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.092$
$S = 1.06$
1630 reflections
125 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0464P)^2 + 0.368P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.010 (2)

Table 1
Selected geometric parameters (Å, °).

Ni1—N7	2.095 (2)	N3—N2	1.183 (3)
Ni1—N5	2.124 (2)	N2—N1	1.160 (3)
Ni1—N3	2.131 (2)		
N7—Ni1—N5^{i}	88.8 (1)	N7—Ni1—N3	87.9 (1)
N7—Ni1—N5	91.2 (1)	N5—Ni1—N3	90.4 (1)
N7—Ni1—N3^{i}	92.1 (1)	N2—N3—Ni1	121.28 (17)
N5—Ni1—N3^{i}	89.6 (1)	N1—N2—N3	177.9 (3)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N6—H6B···N3^{i}	0.86	2.06	2.858 (3)	153
N4—H4B···N1^{ii}	0.86	2.09	2.929 (4)	165

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

All H atoms were generated geometrically and were constrained to ride on their parent atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1994); software used to prepare material for publication: *SHELXL*97.

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References

Arriortua, M. I., Cortes, A. R., Lezama, L., Rojo, T., Solans, X. & Font-Bardia, M. (1990). *Inorg. Chim. Acta*, **174**, 263–269.
Becalska, A., Batchelor, J., Hill, R. H. & Palmer, B. J. (1992). *Inorg. Chem.* **31**, 3118–3123.
Cortes, A. R., Ruiz de Larramendi, J. I., Lezama, L., Urtiaga, K. & Arriortua, M. I. (1992). *J. Chem. Soc. Dalton Trans.* pp. 2723–2728.
Enemark, J. H. (1971). *Inorg. Chem.* **9**, 1952–1957.
Escuer, A., Vicente, R., Ribas, J. & Solans, X. (1995). *Inorg. Chem.* **34**, 1793–1798.

Escuer, A., Vicente, R., Salah, El Fallah, M. S., Solans, X. & Font-Bardia, M. (1996). *Inorg. Chem. Acta*, **247**, 85–91.
Ribas, J., Monfort, M., Bastos, C., Diaz, C. & Solans, X. (1993). *Inorg. Chem.* **32**, 3557–3561.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Siemens (1994). *SAINT* (Version 4.0) and *SHELXTL* (Version 5). Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART*. Version 4.0. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Vicente, R., Escuer, A., Ribas, J., El Fallah, M. S., Solans, X. & Font-Bardia, M. (1993). *Inorg. Chem.* **32**, 1920–1924.
Vicente, R., Escuer, A., Ribas, J., El Fallah, M. S., Solans, X. & Font-Bardia, M. (1995). *Inorg. Chem.* **34**, 1278–1281.