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Tetrakis(1*H*-imidazole-κN^3)nickel(II) dinitrate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.040
wR factor = 0.106
Data-to-parameter ratio = 15.4

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

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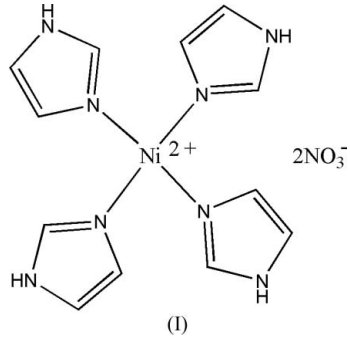
In the title mononuclear nickel(II) complex, $[Ni(C_3H_4N_2)_4](NO_3)_2$, the Ni^{II} atom is four-coordinated in a square-planar geometry by four N atoms from four imidazole ligands. The nitrate anions are linked to the nickel(II) complex cations through intermolecular N—H···O hydrogen bonds.

Comment

Nickel(II) complexes with multidentate ligands have received much attention in recent years (Marganian *et al.*, 1995). Some of the complexes have been found to have pharmacological and catalytic properties (Harrop *et al.*, 2003; Brückner *et al.*, 2000). Nickel is present in the active sites of several important classes of metalloproteins, as either a homodinuclear or a heterodinuclear species. As part of a project to further develop the coordination chemistry of such nickel complexes, the title nickel(II) complex, (I), is reported here.



(I)

The asymmetric unit of (I) contains a mononuclear nickel(II) complex cation and two nitrate anions (Fig. 1). The Ni^{II} atom in (I) is coordinated by four N atoms from four imidazole ligands, forming a four-coordinate square-planar geometry. All the bond lengths and angles (Table 1) involving Ni are comparable with the values reported for similar nickel(II) complexes (Povse *et al.*, 1998; Perec *et al.*, 1999; Spek *et al.*, 1988). Atoms O1 and O6 lie 2.515 (5) and 2.578 (6) Å, respectively, from Ni1. In the crystal structure, the nitrate anions are linked to the nickel(II) complex cations through intermolecular N—H···O hydrogen bonds (Table 2 and Fig. 2).

Experimental

Imidazole (1.0 mmol, 63.2 mg) and $Ni(NO_3)_2{\cdot}6H_2O$ (0.5 mmol, 145.4 mg) were dissolved in methanol (100 ml). The mixture was stirred at room temperature for about 1 h, giving a red solution. After allowing the solution to stand in air for 8 d, red block-shaped crystals were formed.

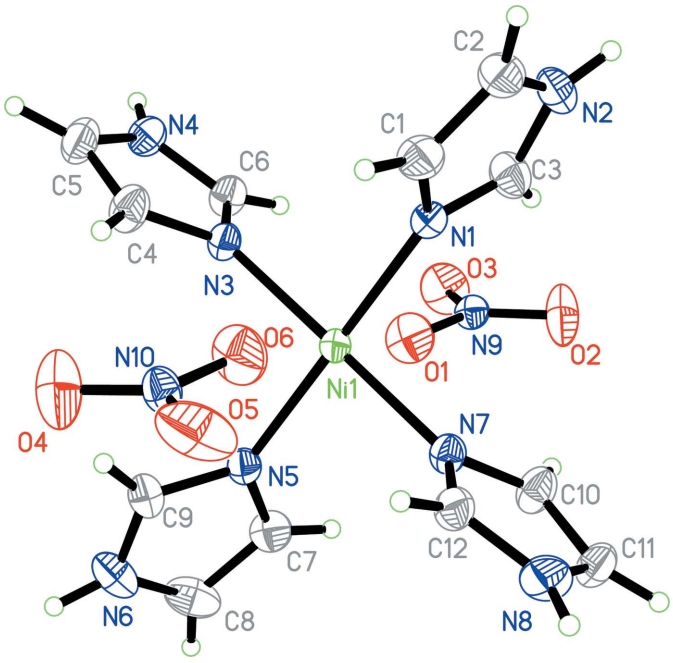


Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

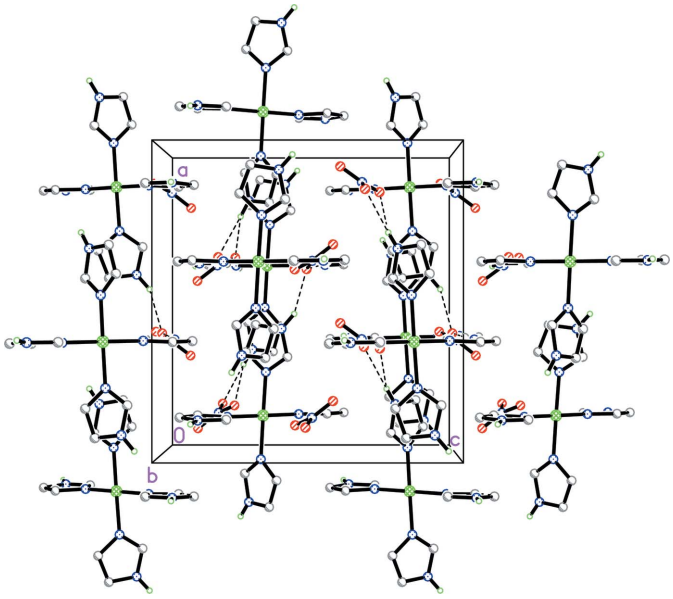


Figure 2
The crystal packing of (I). C-bound H atoms have been omitted. Dashed lines indicate hydrogen bonds.

Crystal data

$[Ni(C_3H_4N_2)_4](NO_3)_2$
M_r = 455.06
Orthorhombic, $Pna2_1$
a = 13.861 (2) Å
b = 9.793 (3) Å
c = 13.372 (2) Å
V = 1815.1 (7) Å^3
Z = 4
D_x = 1.665 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.13 mm^{-1}
T = 298 (2) K
Block, red
0.32 × 0.28 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.715, T_{max} = 0.751
12776 measured reflections
4062 independent reflections
2724 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 28.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.106
S = 1.02
4062 reflections
263 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 1.0722P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack (1983), 1771 Friedel pairs
Flack parameter: 0.27 (3)

Table 1
Selected geometric parameters (Å, °).

Ni1—N7	1.988 (5)	Ni1—N1	2.009 (3)
Ni1—N5	2.003 (3)	Ni1—N3	2.014 (5)
N7—Ni1—N5	89.7 (2)	N7—Ni1—N3	179.4 (2)
N7—Ni1—N1	90.2 (2)	N5—Ni1—N3	89.9 (2)
N5—Ni1—N1	178.8 (2)	N1—Ni1—N3	90.2 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3^{i}	0.86	2.22	2.953 (6)	142
N2—H2···O1^{i}	0.86	2.55	3.361 (7)	158
N2—H2···N9^{i}	0.86	2.70	3.542 (6)	168
N4—H4···O5^{ii}	0.86	2.12	2.808 (8)	137
N6—H6···O5^{iii}	0.86	2.15	2.939 (7)	152
N6—H6···O2^{iv}	0.86	2.62	3.189 (8)	124
N8—H8···O3^{v}	0.86	2.07	2.787 (7)	140

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

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N). The value of the Flack parameter suggests some degree of inversion twinning; attempts to refine the structure in the centrosymmetric space group *Pnma* (non-standard setting of *Pnma*) were unsuccessful.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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