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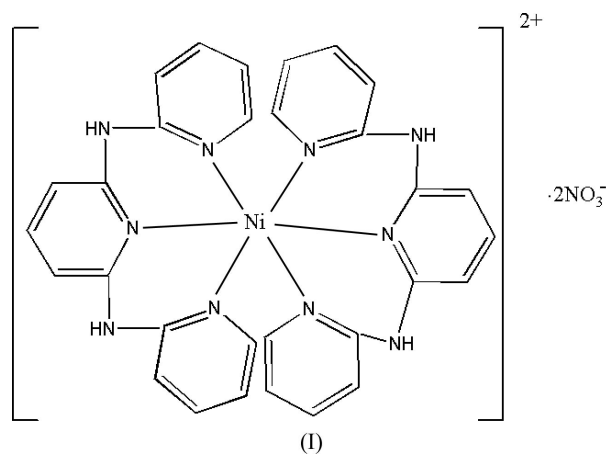
Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.051
 wR factor = 0.148
Data-to-parameter ratio = 12.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis[2,6-bis(2-pyridylamino)pyridine]nickel(II)
dinitrateIn the title complex, $[\text{Ni}(\text{C}_{15}\text{H}_{13}\text{N}_5)_2](\text{NO}_3)_2$, the Ni^{II} ion is located on a twofold axis and is chelated by two tridentate 2,6-bis(2-pyridylamino)pyridine ligands in an octahedral geometry.

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Comment

Transition metal complexes with polypyridylamine ligands have aroused great interest because of their diverse structures and special optical and electromagnetic properties (Xu *et al.*, 2004). The tripyridyldiamine (tpdaH₂) ligand usually exhibits donor and acceptor properties and can be used as a chelating ligand (Jing *et al.*, 2000). A series of polynuclear metal chain complexes has been successfully synthesized and characterized (Sheu *et al.*, 1996; Shieh *et al.*, 1997; Chang *et al.*, 1999). In our current work, we originally attempted to synthesize a complex featuring Ni metal chains by reaction of the Ni^{II} ion with tripyridyldiamine (tpdaH₂); however, the only product obtained was the mononuclear Ni title complex, (I). We report here its synthesis and crystal structure.The crystal structure of (I) consists of Ni^{II} complex cations and nitrate anions (Fig. 1). The Ni^{II} ion is located on a twofold axis and is chelated by two tpdaH₂ ligands in an octahedral geometry, coordinated by six N atoms from two tpdaH₂ ligands. The tpdaH₂ ligands are coordinated meridionally, with the peripheral N1 and N5 atoms in *trans* positions and with N3 *trans* to its symmetry-equivalent. The coordination bond lengths and angles at the Ni^{II} atom are given in Table 1.In (I), the two N atoms of both NH groups of the tpdaH₂ ligands and O atoms of the nitrate anions are linked together by classical N—H···O hydrogen bonds (Table 2), which stabilize the crystal structure. The hydrogen bonds link the ions into an infinite two-dimensional network (Fig. 2).

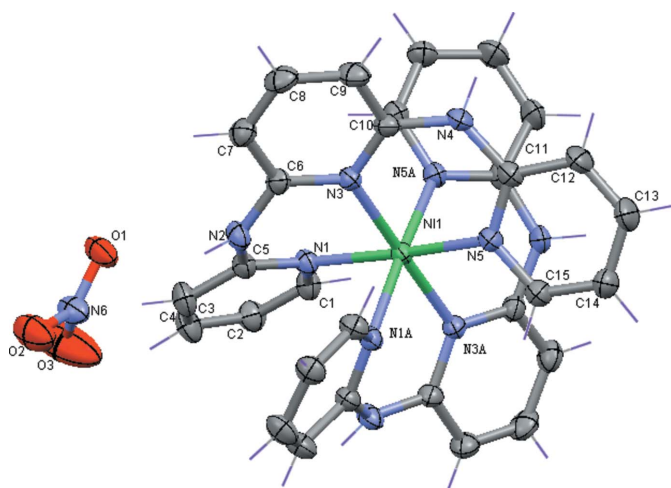


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids; H atoms are indicated only by the C—H bonds as thin lines. Atoms N1A, N3A, N5A and all other unlabelled atoms have the symmetry code $(-x, y, \frac{1}{2} - z)$.

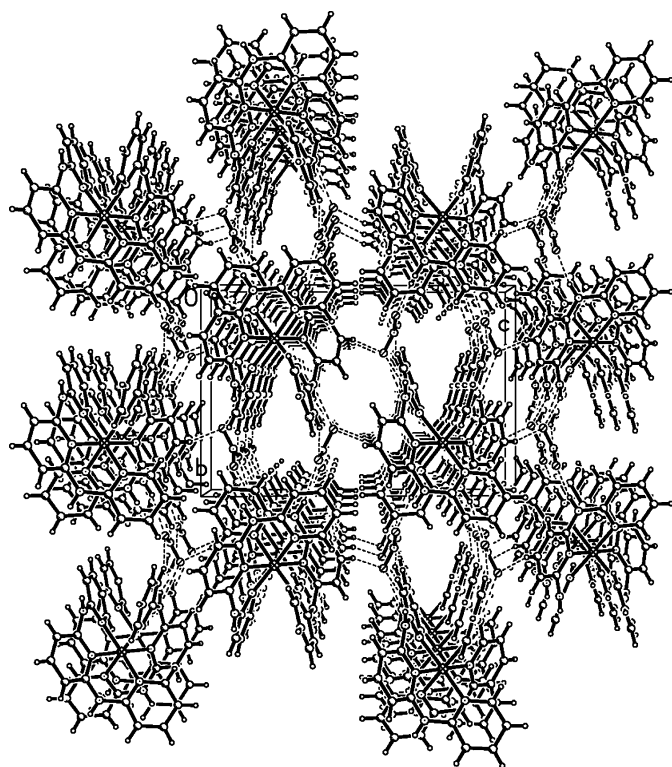


Figure 2
The packing of (I), viewed along the *a* axis, with hydrogen bonds shown as dashed lines.

Experimental

Tripyridylamine (0.08 g), NiCl₂ (0.18 g) and NaNO₃ (0.25 g) were added to a flask and stirred vigorously for 30 min in dry methanol (20 ml). The mixture was then transferred to a Teflon reactor and kept at 383 K for 7 d. Single crystals suitable for X-ray diffraction analysis were obtained.

Crystal data

[Ni(C₁₅H₁₃N₅)₂](NO₃)₂
M_r = 709.34
 Monoclinic, *P*2₁/*c*
a = 8.2138 (12) Å
b = 11.2601 (16) Å
c = 16.790 (2) Å
 β = 93.277 (2)°
V = 1550.4 (4) Å³

Z = 2
D_x = 1.520 Mg m⁻³
 Mo *K*α radiation
 μ = 0.69 mm⁻¹
T = 296 (2) K
 Block, green
 0.35 × 0.14 × 0.13 mm

Data collection

Bruker APEX-II area-detector
 diffractometer
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
T_{min} = 0.795, *T_{max}* = 0.918

7719 measured reflections
 2759 independent reflections
 2318 reflections with *I* > 2σ(*I*)
R_{int} = 0.027
 θ_{max} = 25.1°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.051
wR (*F*²) = 0.148
S = 1.00
 2759 reflections
 222 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0783P)^2 + 1.716P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.93 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.73 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Ni1—N3	2.073 (3)	Ni1—N1	2.083 (3)
Ni1—N5	2.083 (3)		
N3—Ni1—N3 ⁱ	179.33 (14)	N3—Ni1—N1 ⁱ	93.00 (10)
N3—Ni1—N5 ⁱ	92.18 (11)	N5—Ni1—N1 ⁱ	88.50 (11)
N3—Ni1—N5	87.35 (11)	N3—Ni1—N1	87.47 (10)
N3 ⁱ —Ni1—N5	92.18 (10)	N5—Ni1—N1	174.62 (10)
N5 ⁱ —Ni1—N5	93.18 (15)	N1—Ni1—N1 ⁱ	90.30 (15)

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

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N2—H2A···O1	0.86	2.12	2.911 (4)	153
N4—H4A···O3 ⁱ	0.86	2.34	3.170 (6)	163
N4—H4A···O2 ⁱ	0.86	2.40	3.109 (5)	140

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

H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H = 0.93, N—H = 0.86 Å and *U_{iso}*(H) = 1.2*U_{eq}*(C,N).

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2; data reduction: APEX2; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

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