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## Structure Reports

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## Key indicators

Single-crystal X-ray study
$T=293 \mathrm{~K}$
Mean $\sigma(\mathrm{C}-\mathrm{C})=0.008 \AA$
$R$ factor $=0.061$
$w R$ factor $=0.099$
Data-to-parameter ratio $=13.5$
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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# Tris(3,3'-diamino-2,2'-bipyridine)nickel(II) dinitrate 

In the title complex, $\left[\mathrm{Ni}\left(\mathrm{C}_{10} \mathrm{H}_{10} \mathrm{~N}_{4}\right)_{3}\right]\left(\mathrm{NO}_{3}\right)_{2}$, the cation has crystallographic $R 32$ symmetry while the anion lies on a threefold axis. In the cation, the $\mathrm{Ni}^{\mathrm{II}}$ atom is coordinated by six N atoms from three $6,6^{\prime}$-diamino-2, $2^{\prime}$-bipyridine ligands. In the crystal structure, a two-dimensional network is formed via intermolecular $\mathrm{N}-\mathrm{H} \cdots \mathrm{O}$ hydrogen bonds.

## Comment

2,2'-Bipyridine and its derivatives are very useful ligands from which a great number of complexes have been synthesized. Some of these complexes have been used in dye-sensitized solar cells (Kuang et al., 2006; Ferrere, 2002). We have an interest in complexes containing bipyridine and its derivatives as ligands, and have synthesized a series of complexes with $6,6^{\prime}$-diamino-2, $2^{\prime}$-bipyridine as ligand. We report here the structure of the Ni complex, (I) (Fig. 1).


The $\mathrm{Ni}^{\mathrm{II}}$ atom, located on the intersection of a threefold and three twofold axes, is coordinated in a distorted octahedral $\mathrm{ZnN}_{6}$ geometry (Table 1). In the 6,6'-diamino-2,2'-bipyridine ligands, which have twofold rotation symmetry, each pyridine ring is essentially planar with a maximum deviation of 0.068 (4) $\AA$ for atom C5; the dihedral angle between the two pyridine rings is 32.4 (3) ${ }^{\circ}$. This deviation from planarity is expected in terms of steric relief. The anion lies on a threefold axis. In the crystal structure, intermolecular $\mathrm{N}-\mathrm{H} \cdots \mathrm{O}$ hydrogen bonds (Table 2) connect cations and anions, forming a two-dimensional network.

## Experimental

$\mathrm{Ni}\left(\mathrm{NO}_{3}\right)_{2} \cdot 6 \mathrm{H}_{2} \mathrm{O}(0.0316 \mathrm{~g}, 0.109 \mathrm{mmol})$ in $\mathrm{H}_{2} \mathrm{O}(10 \mathrm{ml})$ was added to $6,6^{\prime}$-diamino-2, $2^{\prime}$-bipyridine ( $0.0101 \mathrm{~g}, 0.0542 \mathrm{mmol}$ ) in acetonitrile
$(5 \mathrm{ml})$, and the solution was stirred for a few minutes. Yellow crystals of (I) were obtained after allowing the solution to stand at room temperature for one week. The infrared stretching vibrations of the pyridine ring and amino groups appeared at $1638 \mathrm{~cm}^{-1}, 1465 \mathrm{~cm}^{-1}$ and $1384 \mathrm{~cm}^{-1}$.

## Crystal data

$\left[\mathrm{Ni}\left(\mathrm{C}_{10} \mathrm{H}_{10} \mathrm{~N}_{4}\right)_{3}\right]\left(\mathrm{NO}_{3}\right)_{2}$
$M_{r}=741.39$
$\mathrm{Trigonal}, R 32$
$a=14.537(2) \AA$
$c=13.125(4) \AA$
$V=2402.2(9) \AA^{3}$
$Z=3$

## Data collection

Bruker Smart APEX CCD diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan
SADABS (Sheldrick, 1996)
$T_{\text {min }}=0.917, T_{\text {max }}=0.967$

## Refinement

Refinement on $F^{2}$
$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.061$
$w R\left(F^{2}\right)=0.099$
$S=1.12$
1056 reflections
78 parameters
H -atom parameters constrained
$D_{x}=1.537 \mathrm{Mg} \mathrm{m}^{-3}$
Mo $K \alpha$ radiation
$\mu=0.68 \mathrm{~mm}^{-1}$
$T=293$ (2) K
Prism, yellow
$0.13 \times 0.13 \times 0.05 \mathrm{~mm}$

4515 measured reflections 1056 independent reflections 890 reflections with $I>2 \sigma(I)$
$R_{\text {int }}=0.088$
$\theta_{\text {max }}=26.0^{\circ}$
$w=1 /\left[\sigma^{2}\left(F_{\mathrm{o}}^{2}\right)+(0.0322 P)^{2}\right]$
where $P=\left(F_{\mathrm{o}}{ }^{2}+2 F_{\mathrm{c}}^{2}\right) / 3$
$(\Delta / \sigma)_{\text {max }}<0.001$
$\Delta \rho_{\text {max }}=0.64 \mathrm{e}^{\AA^{-3}}$
$\Delta \rho_{\min }=-0.35$ e $\AA^{-3}$
Absolute structure: Flack (1983),
462 Friedel pairs
Flack parameter: 0.09 (4)

Table 1
Selected geometric parameters $\left(\AA^{\circ},{ }^{\circ}\right)$.

| Ni1-N1 | 2.081 (3) |  |  |
| :---: | :---: | :---: | :---: |
| $\mathrm{N} 1{ }^{\text {i }}-\mathrm{Ni} 11-\mathrm{N} 1^{\text {ii }}$ | 172.7 (3) | $\mathrm{N} 1{ }^{\text {ii }}-\mathrm{Ni} 1-\mathrm{N} 1$ | 96.18 (12) |
| $\mathrm{N} 1{ }^{\mathrm{i}}$ - Ni1-N1 | 78.6 (3) | $\mathrm{N} 1{ }^{\text {i }}-\mathrm{Ni} 1-\mathrm{N} 1^{\text {iii }}$ | 89.5 (2) |
| Symmetry codes: <br> (i) $-y+1, x-y+1, z$ | $\begin{equation*} +\frac{2}{3},-x \tag{ii} \end{equation*}$ | $-z+\frac{1}{3}$ | $+1, z ; \quad \text { (iii) }$ |

Table 2
Hydrogen-bond geometry ( $\AA{ }^{\circ},{ }^{\circ}$ ).

| $D-\mathrm{H} \cdots A$ | $D-\mathrm{H}$ | $\mathrm{H} \cdots A$ | $D \cdots A$ | $D-\mathrm{H} \cdots A$ |
| :--- | :--- | :--- | :--- | :--- |
| $\mathrm{~N} 2-\mathrm{H} 2 B \cdots \mathrm{~N}^{\text {i }}$ | 0.86 | 2.37 | $2.829(9)$ | 114 |

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



Figure 1
The cation and anion of (I), showing the atom-numbering scheme with displacement ellipsoids drawn at the $30 \%$ probability level. [Symmetry codes: (i) $-x+\frac{2}{3},-x+y+\frac{1}{3},-z+\frac{1}{3}$; (ii) $-y+1, x-y+1, z$; (iii) $-x+y$, $-x+1, z ;$ (iv) $y-\frac{1}{3}, x+\frac{1}{3},-z+\frac{1}{3}$; (v) $x-y+\frac{2}{3},-y+\frac{4}{3},-z+\frac{1}{3}$; (vi) $-y, x-y$, $z$; (vii) $-x+y,-x, z$.]

The H atoms were placed in calculated positions and refined in the riding-model approximation, with $\mathrm{C}-\mathrm{H}=0.93 \AA, U_{\text {iso }}(\mathrm{H})=1.2_{\text {eq }}(\mathrm{C})$; $\mathrm{N}-\mathrm{H}=0.86 \AA, U_{\text {iso }}(\mathrm{H})=1.2_{\text {eq }}(\mathrm{N})$.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2001); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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