Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Tris(3,3′-diamino-2,2′-bipyridine)manganese(II) dinitrate

**Jing-Min Shi,* Ju-Na Chen and Lian-Dong Liu**

Department of Chemistry, Shandong Normal University, Jinan 250014, People's Republic of China

Correspondence e-mail: shijingmin@beelink.com

**Key indicators**

Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.006 Å
*R* factor = 0.038
*wR* factor = 0.089
Data-to-parameter ratio = 7.9

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

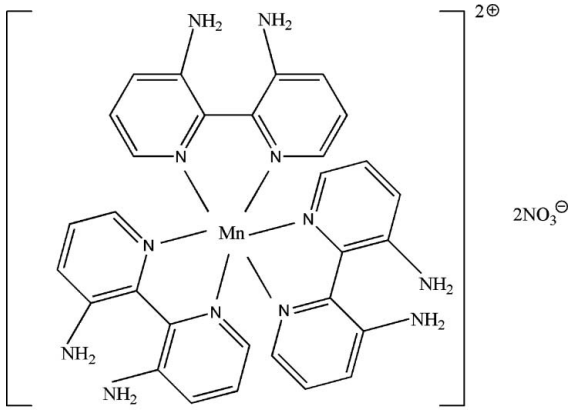
© 2006 International Union of Crystallography
All rights reserved

Received 21 July 2006
Accepted 8 August 2006

In the title complex, $[Mn(C_{10}H_{10}N_4)_3](NO_3)_2$, the six-coordinate $Mn^{II}$ atom is located on the intersection of one threefold and three twofold axes, while the nitrate anion lies on a threefold axis. In the crystal structure, a two-dimensional network is formed *via* intermolecular N—H···N and N—H···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 dye-sensitized solar cells involve complexes of derivatives of 2,2′-bipyridine as ligand (Kuang *et al.*, 2006). We have an interest in complexes containing bipyridine and its derivatives as ligands and have synthesized an $Ni^{II}$ complex with 3,3′-diamino-2,2′-bipyridine as ligand (Min *et al.*, 2006). We report here the structure of the Mn complex, (I) (Fig. 1).




(I)

The $Mn^{II}$ atom, located on the intersection of one threefold and three twofold axes, is coordinated in a distorted octahedral $MnN_6$ geometry (Table 1) and the nitrate anion lies on a threefold axis. In the 3,3′-diamino-2,2′-bipyridine ligands, each pyridine ring is essentially planar, with a maximum deviation of 0.051 (3) Å for atom C1; the dihedral angle between the two pyridine rings is 37.28 (17)°, which is larger than that of the $Ni^{II}$ complex of 32.4 (3)°. Just as in the $Ni^{II}$ complex, the deviation from planarity is also expected in terms of steric relief. In the crystal structure, intermolecular N—H···N and N—H···O hydrogen bonds (Table 2) connect cations and anions, forming a two-dimensional network.

## Experimental

$Mn(NO_3)_2·6H_2O$ (0.0332 g, 0.116 mmol) in $H_2O$ (10 ml) was added to 3,3′-diamino-2,2′-bipyridine (0.0435 g, 0.234 mmol) in acetonitrile

(5 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 two weeks.

*Crystal data*

$[Mn(C_{10}H_{10}N_4)_3](NO_3)_2$
$M_r$ = 737.62
Trigonal, *R*32
*a* = 14.7149 (16) Å
*c* = 13.229 (3) Å
*V* = 2480.8 (7) Å$^3$
*Z* = 3
$D_x$ = 1.481 Mg m$^{-3}$
Mo *K*α radiation
μ = 0.47 mm$^{-1}$
*T* = 298 (2) K
Prism, yellow
0.38 × 0.21 × 0.20 mm

*Data collection*

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.843, $T_{max}$ = 0.913
4198 measured reflections
615 independent reflections
572 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.049
$\theta_{max}$ = 26.0°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.089
*S* = 1.11
615 reflections
78 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$
Absolute structure: Flack (1983), with 480 Friedel pairs
Flack parameter: 0.47 (5)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Mn1—N1 | 2.237 (2) | N2—C2 | 1.371 (5) |
| N1—C5 | 1.326 (4) | N3—O1 | 1.237 (2) |
| N1—C1 | 1.344 (4) | | |
| $N1^{i}$—Mn1—$N1^{ii}$ | 92.53 (14) | $N1^{ii}$—Mn1—$N1^{iii}$ | 97.44 (8) |
| $N1^{i}$—Mn1—$N1^{iii}$ | 167.54 (14) | $N1^{iii}$—Mn1—$N1^{iv}$ | 73.76 (12) |

Symmetry codes: (i) $-x+y+1, -x+2, z$; (ii) $x-y+1, -y+2, -z$; (iii) $y, x, -z$; (iv) $-y+2, x-y+1, z$.

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*B*···$N2^{ii}$ | 0.86 | 2.41 | 2.850 (7) | 113 |
| N2—H2*A*···$O1^{v}$ | 0.86 | 2.14 | 2.984 (4) | 167 |

Symmetry codes: (ii) $x-y+1, -y+2, -z$; (v) $-y+1, x-y+1, z$.

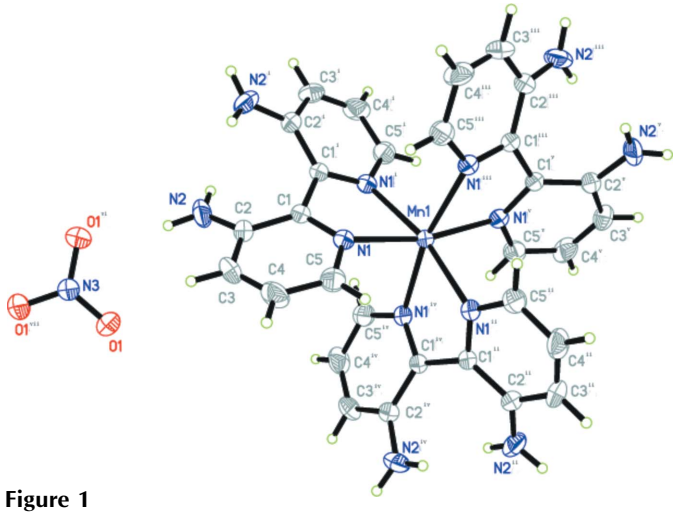



**Figure 1**
The structure of (I), showing the atom-numbering scheme, with displacement ellipsoids drawn at the 30% probability level. [Symmetry codes: (i) $x-y+1, -y+2, -z$; (ii) $-y+2, x-y+1, z$; (iii) $-x+y+1, -x+2, z$; (iv) $y, x, -z$; (v) $-x+2, -x+y+1, -z$; (vi) $-y+1, x-y+1, z$; (vii) $-x+y, -x+1, z$.]

H atoms were positioned geometrically, with N—H = 0.86 Å and C—H = 0.93 Å, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C,N)$. The Flack parameter of 0.47 (5) (Flack, 1983) suggests that the crystal is an inversion twin.

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*.

The authors thank the Natural Science Foundation of Shandong Province, China (grant No. Y2005B25).

## References

Bruker (1997). *SMART* (Version 5.6) and *SAINT* (Version 5. A06). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Kuang, D., Klein, C., Snaith, H. J., Moser, J.-E., Humphry-Baker, R., Comte, P., Zakeeruddin, S. M. & Gratzel, M. (2006). *Nano Lett.* **6**, 769–773.
Min, S. J., Na, C. J. & Dong, L. L. (2006). *Acta Cryst.* E**62**, m1810–m1811.
Sheldrick, G. M. (1996). *SADABS*. Version 2.10. University of Göttingen, Germany.