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Diazidobis(2,2′-bipyridine)manganese(II)

Ya-Qian Cheng,* Mao-Lin Hu, Sai-Rong Fan and Wei Zhang

Department of Chemistry and Material Science, Wenzhou Normal College, Wenzhou 325027, People's Republic of China

Correspondence e-mail:
hu403cn@yahoo.com.cn

In the title compound, $[Mn(N_3)_2(C_{10}H_8N_2)_2]$, the Mn atom, on a twofold rotation axis, is chelated by the two heterocyclic ligands, with the two azide groups in *cis* positions in the distorted octahedral coordination.

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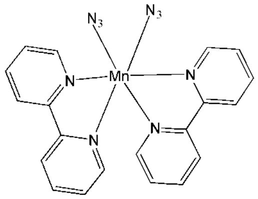
Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.005 Å
R factor = 0.059
wR factor = 0.138
Data-to-parameter ratio = 12.7

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

Comment

Considerable efforts have recently been concentrated on the synthesis and properties of complexes bridged by the azide anion, due to their intriguing structural diversity, and potential functions as models for metalloenzymes and ferromagnetic or antiferromagnetic interactions (Aebersold *et al.*, 1998; Baffert *et al.*, 2001). The azide anion can bind to metal ions in versatile modes: as a terminal ligand *via* one nitrogen donor, as a bridge in the $\mu_{1,1}$ manner *via* one nitrogen donor, and in the $\mu_{1,3}$ manner *via* both of the terminal *N*-donor atoms (Sheppard *et al.*, 1996). In our previous work, we have reported two monomeric complexes (Cheng & Hu, 2003; Cheng, Liu *et al.*, 2002) and a dimeric complex (Cheng, Hu *et al.*, 2002). Extending this research, we report here another new monomeric complex, namely diazidobis(2,2′-bipyridine)-manganese(II), (I).



(I)

In (I), two 2,2′-bipyridine (bpy) molecules, one manganese(II) cation and two azide anions constitute a monomeric unit, with Mn lying on a twofold rotation axis; the metal atom adopts an MnN_6 octahedral geometry defined by four N atoms from two bpy ligands and two N atoms from two azide anions that occupy *cis* positions (Fig. 1). The basal plane [N2, N2^{i}, N3 and N3^{i}; symmetry code: (i) $-x, y, \frac{3}{2} - z$] consists of two azide N atoms and two bpy N atoms, with bond lengths in the range 2.148 (3)–2.274 (3) Å. The apical positions are occupied by the other two bpy N atoms, with equal bond distances of 2.322 (3) Å and an angle of 160.42 (15)°. Thus, the six-coordinate geometry of the manganese center can best be described as distorted octahedral, and is not significantly different from that found in the 2,2-bipyridine analog, which crystallizes as a monohydrate (Urtiaga *et al.*, 1995).

Experimental

A mixture of manganese sulfate (1 mmol, 0.22 g), 2,2′-bipyridine (2 mmol, 0.31 g) and sodium azide (2 mmol, 0.13 g) in 50 ml of a

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water and ethanol mixture (1:2 *v*:*v*) was stirred for several hours at room temperature. The mixture was filtered and red crystals separated from the filtrate after two weeks.

Crystal data

$[Mn(N_3)_2(C_{10}H_8N_2)_2]$
$M_r = 451.37$
Orthorhombic, *Pbcn*
$a = 14.5978$ (10) Å
$b = 8.1794$ (6) Å
$c = 16.9523$ (12) Å
$V = 2024.1$ (2) Å^3
$Z = 4$
$D_x = 1.481$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 324 reflections
$\theta = 2.5$–$22.0°$
$\mu = 0.68$ mm^{-1}
$T = 273$ (2) K
Prism, red
0.42 × 0.29 × 0.28 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.762$, $T_{max} = 0.832$
13540 measured reflections

1787 independent reflections
1751 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.1°$
$h = -17 \rightarrow 17$
$k = -9 \rightarrow 9$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.138$
$S = 1.34$
1787 reflections
141 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 2.3037P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

H atoms were positioned geometrically and allowed to ride on their parent atoms at a distance of 0.93 Å, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); 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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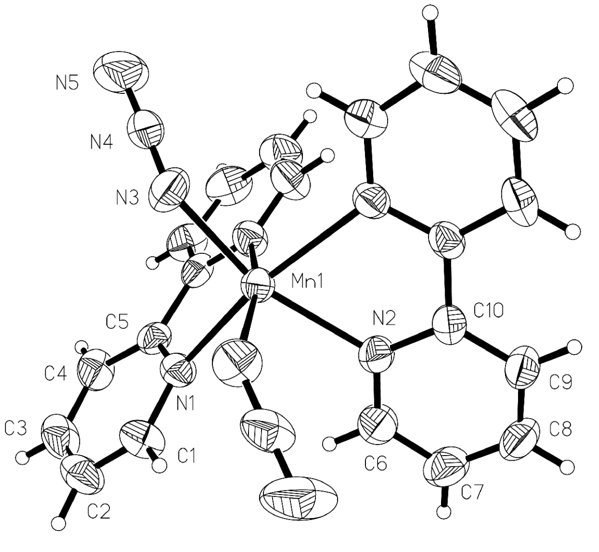

Figure 1
The molecular structure of (I), with the atom numbering, showing displacement ellipsoids at the 50% probability level.

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