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Aquaazidobis(2,2′-bipyridine)manganese(II) perchlorate

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Key indicators

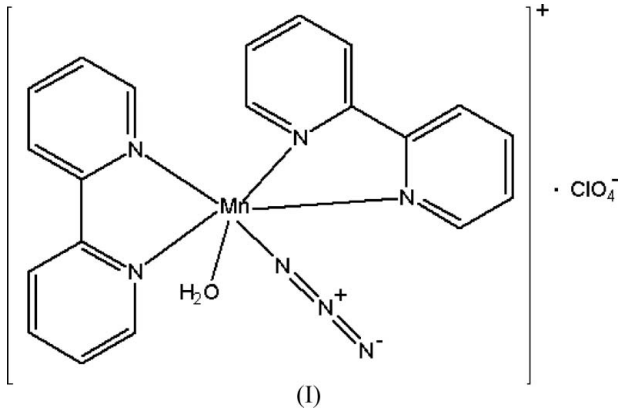
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.099
Data-to-parameter ratio = 12.9

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

In the title complex, $[Mn(N_3)(C_{10}H_8N_2)_2(H_2O)]ClO_4$, each Mn atom is surrounded by one O atom from an aqua ligand, one N atom from an azide anion and four N atoms from 2,2′-bipyridine ligands to form a distorted octahedral geometry. In the complex, the perchlorate anion acts as a counter-ion to balance the charge.

Comment

It is known that azide complexes have received intense attention due to their structural and magnetic diversity (Song *et al.*, 2004). The versatility and efficacy of the azide group lies in its functionality as a terminal monodentate or bridging ligand (Gao *et al.*, 2003; Maji *et al.*, 2001; Goher & Mautner, 1999; Escuer *et al.*, 1999; Ribas *et al.*, 1999; Perlepes *et al.*, 2001; Guo & Mak, 1998). We have carried out much work with the azide ligand in the hope of obtaining some azide complexes with one-, two- or three-dimensional networks with strong ferromagnetic or antiferromagnetic behaviour. Here, we report a mononuclear complex with an azide group terminally coordinated to a metal atom, $[Mn(C_{10}H_8N_2)_2(N_3)(H_2O)](ClO_4)$, (I).



(I)

As shown in Fig. 1, the Mn atom of (I) is *cis* six-coordinated by a water molecule, a monodentate azide group and two 2,2′-bipyridine ligands to form a distorted octahedral geometry. The two 2,2′-bipyridine planes are nearly perpendicular to each other, with a dihedral angle of 82.0°. In the equatorial plane, the bond lengths of Mn to N2, N3 and N4 are a little longer than the distance between the Mn atom and atom N5 of the azide (Table 1).

The packing of complex (I) (Fig. 2) shows three types of hydrogen bond (Table 2).

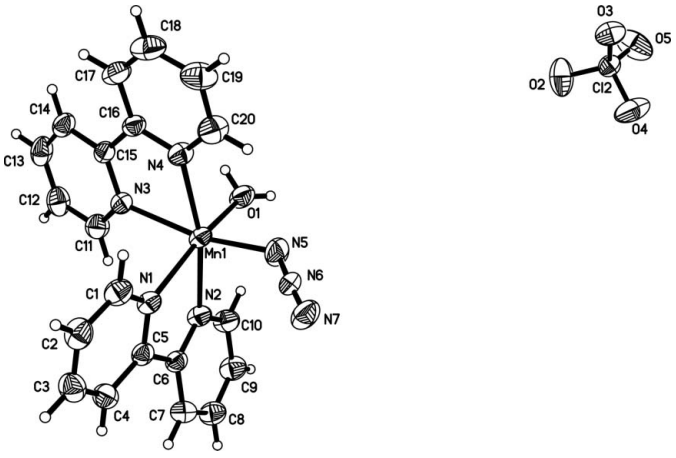


Figure 1
The asymmetric unit of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radii.

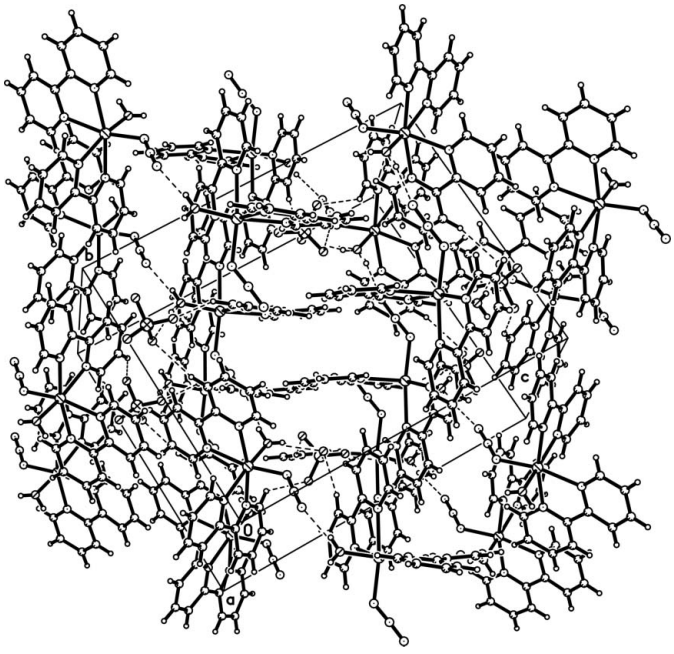


Figure 2
A crystal packing diagram of complex (I). Dashed lines indicate hydrogen bonds.

Experimental

Compound (I) was synthesized in a solution reaction. NaN_3 (0.2 mmol) dissolved in water (2 ml) was added to an aqueous solution (5 ml) of $Mn(ClO_4)_4{\cdot}6H_2O$ (0.1 mmol) with stirring. An ethanol solution (5 ml) of 2,2′-bipyridine (0.2 mmol) was then added to the solution and the mixture was stirred for 6 h. The mixture was then filtered and the resulting clear solution was kept at room temperature to evaporate slowly. After one week, single crystals of (I) suitable for X-ray diffraction were obtained.

Crystal data

$[Mn(N_3)(C_{10}H_8N_2)_2(H_2O)]ClO_4$
M_r = 526.80
Monoclinic, $P2_1/c$
a = 9.0144 (3) Å
b = 14.4325 (5) Å
c = 17.5808 (6) Å
β = 95.570 (2)°
V = 2276.47 (13) Å^3
Z = 4
D_x = 1.537 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.75 mm^{-1}
T = 273 (2) K
Prism, green
0.20 × 0.18 × 0.12 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.865, T_{max} = 0.916
14158 measured reflections
4032 independent reflections
3086 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.099
S = 1.07
4032 reflections
313 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0454P)^2 + 0.628P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0026 (6)

Table 1
Selected geometric parameters (Å, °).

Mn1—N5	2.129 (2)	Mn1—N1	2.269 (2)
Mn1—O1*W*	2.179 (2)	Mn1—N3	2.2695 (19)
Mn1—N4	2.254 (2)	N5—N6	1.171 (3)
Mn1—N2	2.253 (2)	N6—N7	1.156 (3)
N5—Mn1—O1*W*	94.46 (10)	N2—Mn1—N1	72.57 (7)
N5—Mn1—N4	93.54 (9)	N5—Mn1—N3	165.74 (9)
O1*W*—Mn1—N4	92.55 (8)	O1*W*—Mn1—N3	86.05 (8)
N5—Mn1—N2	98.52 (9)	N4—Mn1—N3	72.20 (8)
O1*W*—Mn1—N2	90.73 (8)	N2—Mn1—N3	95.72 (7)
N4—Mn1—N2	167.21 (8)	N1—Mn1—N3	90.87 (7)
N5—Mn1—N1	92.69 (9)	N6—N5—Mn1	133.4 (2)
O1*W*—Mn1—N1	162.65 (8)	N7—N6—N5	177.4 (3)
N4—Mn1—N1	102.76 (8)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···N7^{i}	0.82	1.99	2.802 (3)	169
O1*W*—H1*WB*···O3^{ii}	0.74 (4)	2.18 (4)	2.899 (3)	166 (4)
O1*W*—H1*WB*···Cl1^{ii}	0.74 (4)	2.94 (4)	3.577 (2)	146 (4)

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

Atom H1*WB* was located in a difference Fourier map and refined freely. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å, O—H = 0.82 Å and U_{iso}(H) = 1.2U_{eq}(C,O).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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