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Hexakis(*N*-methyl-1*H*-imidazole-κN^3)manganese(II) dibromide dihydrate

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Key indicators

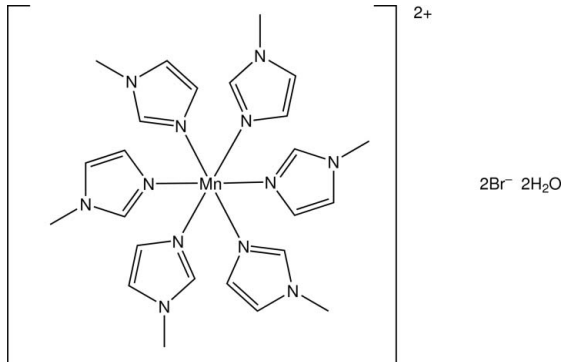
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.023
wR factor = 0.060
Data-to-parameter ratio = 19.5

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

The manganese complex of the title compound, $[Mn(C_4H_6N_2)_6]Br_2{\cdot}2H_2O$, is located on a crystallographic inversion centre. The anions and solvent molecules form a hydrogen-bonded cluster of formulation $Br_2(H_2O)_2$ with graph set $R_4^2(8)$.

Comment

The hexakis(*N*-methylimidazole)manganese(II) complex has been reported in crystal structures with phenylthiolate, phenylperthiolate (Krautscheid *et al.*, 1993) and octasulfide (Dev *et al.*, 1991) as counter-ions. In this paper, the crystal structure of the Mn complex, (I), with bromide as counter-ion and a cocrystallized water molecule is reported. The Mn^{II} ion is located on a crystallographic inversion centre in an octahedral coordination environment. The maximum deviation of the N—Mn—N angles from ideal values is 2.6° (Table 1).



(I)

The crystal packing consists of a checker-board alternation of Mn complexes and $Br_2(H_2O)_2$ clusters in the *bc* plane (see Fig. 2). The bromide ions and water molecules are joined by hydrogen bonds in a cluster which has the primary graph set $R_4^2(8)$ (Bernstein *et al.*, 1995). Geometric details of the hydrogen bonds are given in Table 2.

Experimental

Crystals of (I) were obtained as a side product in a study on the stereochemical influence of the ligand on the structure of manganese(II) complexes (Godbole *et al.*, 2005).

Crystal data

$[Mn(C_4H_6N_2)_6]Br_2{\cdot}2H_2O$
M_r = 743.42
Monoclinic, $P2_1/c$
a = 8.1137 (10) Å
b = 13.6259 (10) Å
c = 16.057 (2) Å
β = 110.993 (11)°
V = 1657.4 (3) Å^3
Z = 2
D_x = 1.490 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.85 mm^{-1}
T = 150 K
Block, colourless
0.40 × 0.40 × 0.20 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ scans and ω scans with κ offset
Absorption correction: multi-scan (*MULABS* in *PLATON*; Spek, 2003)
T_{min} = 0.309, T_{max} = 0.568
42360 measured reflections
3820 independent reflections
3440 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.060
S = 1.03
3820 reflections
196 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0269P)^2 + 1.05P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—N3	2.2546 (14)	Mn1—N23	2.2670 (16)
Mn1—N13	2.2949 (15)		
N3—Mn1—N13	92.60 (5)	N3—Mn1—N23^{i}	88.43 (5)
N3—Mn1—N23	91.57 (5)	N13—Mn1—N23	89.94 (6)
N3—Mn1—N13^{i}	87.40 (5)	N13—Mn1—N23^{i}	90.07 (6)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···Br1^{ii}	0.81 (3)	2.55 (3)	3.3547 (18)	175 (3)
O1—H1B···Br1^{iii}	0.82 (3)	2.50 (3)	3.3160 (18)	176 (2)

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

H atoms bonded to C were placed in calculated positions (C—H = 0.95–0.98 Å), riding on their carrier atoms. The methyl groups were allowed to rotate around the N—Me bond. The coordinates of the water H atoms were determined from a difference Fourier map and were freely refined. U_{iso}(H) = 1.5U_{eq}(water O and methyl C) or 1.2U_{eq}(imidazole C).

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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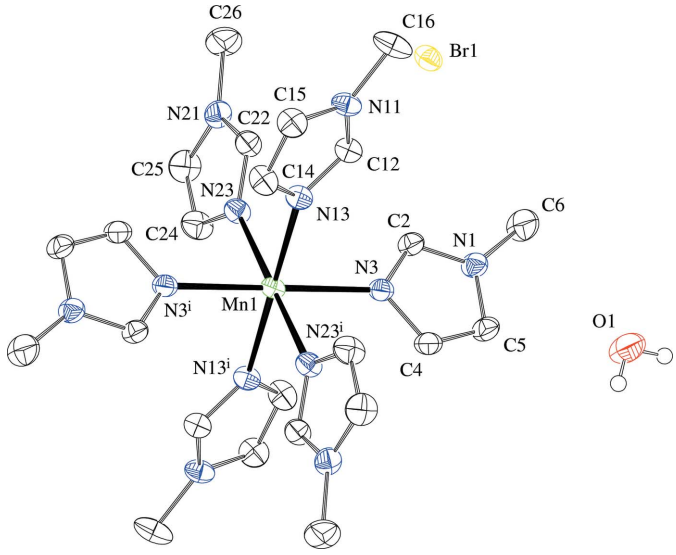

Figure 1
Molecular structure of the title compound (I), with displacement ellipsoids drawn at the 30% probability level. H atoms bonded to C atoms have been omitted for clarity. [Symmetry code: (i) $2-x, -y, 1-z$.]

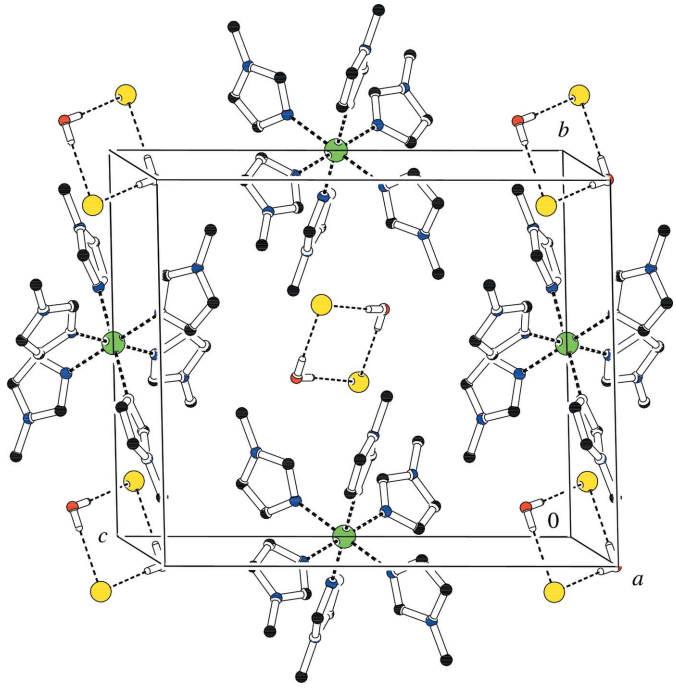

Figure 2
View of the crystal packing down *a*. Dashed lines indicate hydrogen bonds. H atoms bonded to C atoms have been omitted.

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