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A linear supramolecular array of $\{[Mn(H_2O)_2(15\text{-crown-5})]Br_2\}_n$

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Key indicators

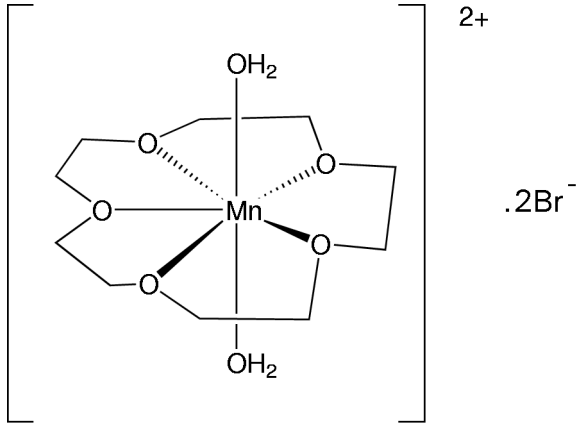
Single-crystal X-ray study
T = 294 K
Mean σ(C—C) = 0.004 Å
R factor = 0.024
wR factor = 0.086
Data-to-parameter ratio = 14.8

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

Diaqua(1,4,7,10,14-pentaoxacyclopentadecane)manganese(II) dibromide, $[Mn(C_{10}H_{20}O_5)(H_2O)_2]Br_2$, prepared in a search for emissive Mn^{II} ions in unusual coordination environments, contains the metal ion encircled by the crown ether ligand, with the water molecules in *trans* axial positions. Hydrogen bonding between these and the Br^- counter-ions forms chains of cations running approximately parallel to **a**.

Comment

Compounds of Mn^{2+} and 15-crown-5 were prepared in search of crystals with emissive Mn^{II} ions in environments other than tetrahedral or octahedral geometries (Reid *et al.*, 1998, 1999). In one of these, $[Mn(H_2O)_2(15\text{-crown-5})]Br_2$, (I), the cation was found to have crystallographically imposed twofold rotation symmetry, with the axis passing through O1, Mn and the midpoint of the C5—C5*A* bond. The cations are arranged in chains approximately parallel to *a* and held together by hydrogen bonding between the water molecules and the Br^- ions.



(I)

Experimental

$MnBr_2{\cdot}4H_2O$ (1 mmol) and a slight excess of 15-crown-5 were dissolved in 40 ml of methanol. Vapor diffusion of diethyl ether into this solution at 293 K afforded pale brown columnar crystals of the title compound in 86% yield. Analysis calculated for $C_{10}H_{24}Br_2MnO_7$: C 25.5, H 5.1, Br 33.9%; found: C 25.3, H 5.1, Br 33.8%.

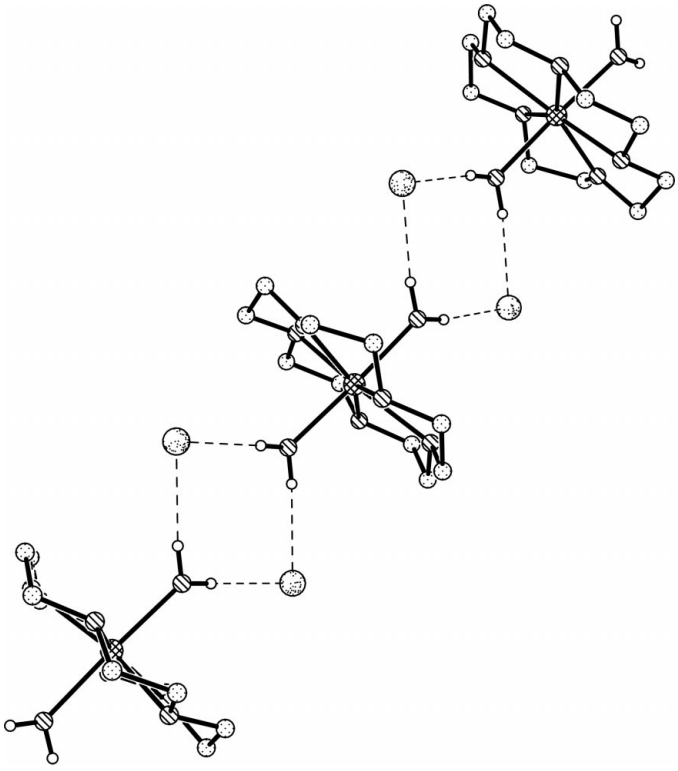


Figure 1
The hydrogen-bonded cation-anion chain.

Crystal data

$[Mn(C_{10}H_{20}O_5)(H_2O)_2]Br_2$
M_r = 471.05
Monoclinic, *C*2/*c*
a = 13.687 (2) Å
b = 15.856 (1) Å
c = 7.7761 (9) Å
β = 97.936 (9)°
V = 1671.4 (5) Å^3
Z = 4
D_x = 1.87 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 25 reflections
θ = 13–17°
μ = 5.6 mm^{-1}
T = 293 K
Column, pale brown
0.50 × 0.40 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: empirical *via* ψ scan (North *et al.*, 1968)
T_{min} = 0.084, T_{max} = 0.196
1780 measured reflections
1644 independent reflections
1362 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 26.0°
h = 0 → 16
k = 0 → 19
l = −9 → 9
3 standard reflections
frequency: 120 min
intensity decay: <1%

Refinement

Refinement on *F*
R = 0.024
wR = 0.086
S = 1.28
1362 reflections
92 parameters
H-atom parameters not refined
$w = 4F_o^2/[\sigma^2(F_o^2) + 0.0016F_o^4]$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H1*W*···Br^{i}	0.88	2.35	3.216 (2)	172
O4—H2*W*···Br	0.89	2.36	3.246 (2)	173

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

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *PROCESS* in *MolEN* (Fair, 1990); program(s) used to solve structure: *SIR* (Burla *et al.*, 1989); program(s) used to refine structure: *LSFM* in *MolEN* (Fair, 1990); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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