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catena-Poly[[[diaquamanganese(II)]bis(μ-1*H*-benzimidazole-5-carboxylato)-κ^2N^3:*O*;κ^2*O*:N^3] dihydrate]

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.028
wR factor = 0.082
Data-to-parameter ratio = 12.8

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

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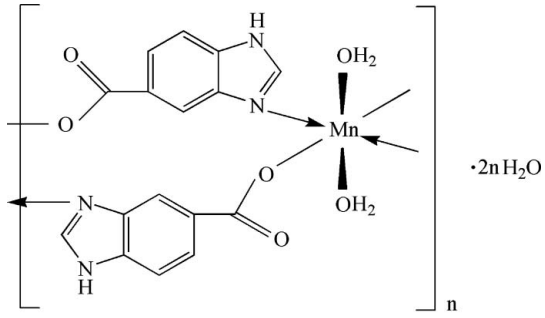
In the crystal structure of the title compound, $\{[Mn(C_8H_5N_2O_2)_2(H_2O)_2]\cdot 2H_2O\}_n$, two 1*H*-benzimidazole-5-carboxylate anions bridge two adjacent water-coordinated Mn cations to furnish a linear chain; the Mn atom lies on a crystallographic inversion centre. Adjacent chains are linked through the Mn cations and the coordinated and uncoordinated water molecules into a three-dimensional network motif.

Comment

An enormous number of transition metal heteroarylcarboxylates having a Lewis basic nitrogen donor have been structurally documented (Allen, 2002). The 5-benzimidazolylcarboxylate ion, by virtue of the position of the carboxylic substituent, could function as a bridging ligand. In the present manganese(II) complex, (I) (Fig. 1), two of the anions link adjacent water-coordinated manganese cations into a chain (Fig. 2). The chain adopts a helical conformation as it propagates by screw-axis operations along the *c* axis of the monoclinic unit cell. Adjacent chains are consolidated into a tightly held three-dimensional network by hydrogen bonds (Fig. 3 and Table 2). The compound has the same structure as the reported cobalt(II) derivative (Liu *et al.*, 2005), which has been described in detail.



(I)

Experimental

The compound was synthesized from manganese dichloride hexahydrate (0.083 g, 0.5 mmol), benzimidazole-5-carboxylic acid (0.162 g, 1.0 mmol), sodium hydroxide (0.04 g, 1.0 mmol), triethylamine (0.5 ml, excess) and water (16 ml). The mixture was heated in a Teflon-lined stainless steel autoclave for 144 h at 423 K. The autoclave was cooled to room temperature over a period of 12 h at 100 K h^{-1}; the compound separated as pale-yellow columnar crystals in about 20% yield.

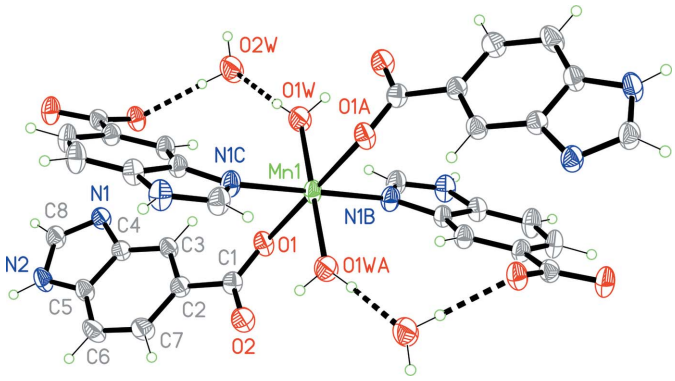


Figure 1
The octahedral geometry of Mn in (I). Displacement ellipsoids are drawn at the 50% probability level and dashed lines indicate hydrogen bonds. [Symmetry code: (A) $1-x, 1-y, 1-z$; (B) $x, 1-y, z-\frac{1}{2}$; (C) $1-x, y, \frac{1}{2}-z$.]

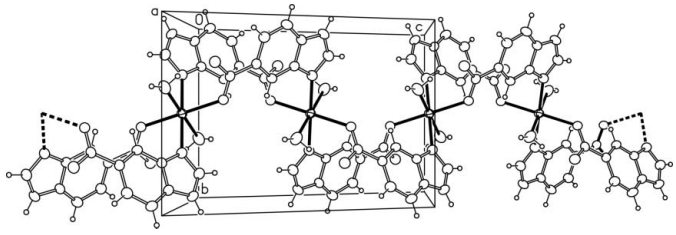


Figure 2
View of the one-dimensional chain in (I), running along the *b* axis. Hydrogen bonds are shown as dashed lines.

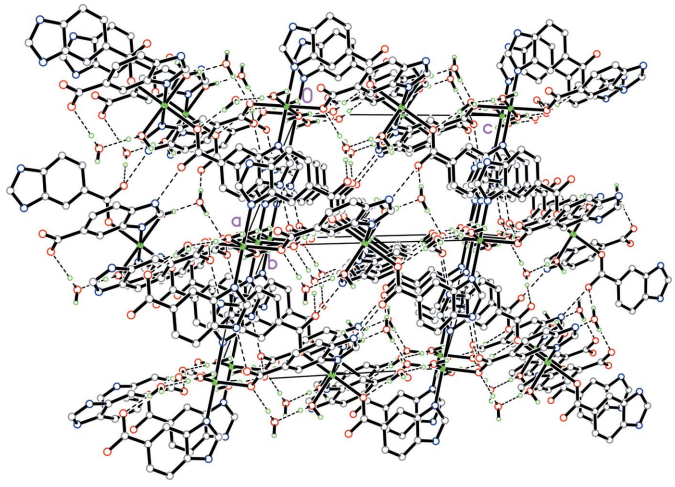


Figure 3
Packing diagram of (I). Hydrogen-bond interactions are shown as dashed lines and only O-bound H atoms are displayed for clarity.

Crystal data

$[Mn(C_8H_5N_2O_2)_2(H_2O)_2]\cdot 2H_2O$
$M_r = 449.28$
Monoclinic, $C2/c$
$a = 16.246\ (2)$ Å
$b = 9.076\ (1)$ Å
$c = 14.198\ (2)$ Å
$\beta = 119.543\ (2)^\circ$
$V = 1821.4\ (4)$ Å^3
$Z = 4$
$D_x = 1.638$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.78$ mm^{-1}
$T = 295\ (2)$ K
Column, light yellow
0.35 × 0.15 × 0.10 mm

Data collection

Bruker SMART 1K area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.707$, $T_{max} = 0.926$
4919 measured reflections
1966 independent reflections
1667 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 27.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.082$
$S = 1.02$
1966 reflections
153 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0518P)^2 + 0.9912P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.222 (1)	Mn1—N1^{i}	2.250 (1)
Mn1—O1*W*	2.189 (1)	Mn1—N1^{ii}	2.250 (1)
O1—Mn1—O1^{iii}	180	O1—Mn1—N1^{ii}	84.43 (5)
O1—Mn1—O1*W*	93.15 (5)	O1*W*—Mn1—O1*W*^{iii}	180
O1—Mn1—O1*W*^{iii}	86.85 (5)	O1*W*—Mn1—N1^{i}	83.93 (5)
O1—Mn1—N1^{i}	95.57 (5)	O1*W*—Mn1—N1^{ii}	96.07 (5)

Symmetry codes: (i) $x, -y+1, z-\frac{1}{2}$; (ii) $-x+1, y, -z+\frac{3}{2}$; (iii) $-x+1, -y+1, -z+1$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2^{iii}	0.84 (1)	1.92 (1)	2.716 (2)	159 (2)
O1*W*—H1*W*2···O2*W*	0.84 (1)	1.87 (1)	2.707 (2)	176 (2)
O2*W*—H2*W*1···O1^{ii}	0.85 (1)	1.92 (1)	2.770 (2)	176 (3)
O2*W*—H2*W*2···O2^{iv}	0.85 (1)	1.98 (1)	2.810 (2)	165 (3)
N2—H2N···O2^{v}	0.85 (1)	1.98 (1)	2.823 (2)	171 (2)

Symmetry codes: (ii) $-x+1, y, -z+\frac{3}{2}$; (iii) $-x+1, -y+1, -z+1$; (iv) $x-\frac{1}{2}, y-\frac{1}{2}, z$; (v) $x, -y+2, z+\frac{1}{2}$.

The C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to $1.2U_{eq}$(C). The water and amine H atoms were located in difference Fourier maps, and were refined with distance restraints giving O—H = 0.84 (1)–0.85 (1) Å [U_{iso}(H) = $1.5U_{eq}$(O)] and N—H = 0.85 (1) Å [U_{iso}(H) = $1.2U_{eq}$(N)].

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: atomic coordinates taken from the Co analogue (Liu *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXL97*.

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