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catena-Poly[[[diaqua(2,2′-diamino-4,4′-bithiazole-κ^2N,N')manganese(II)]-μ-terephthalato-$\kappa^2O:O'$] dihydrate]

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Key indicators

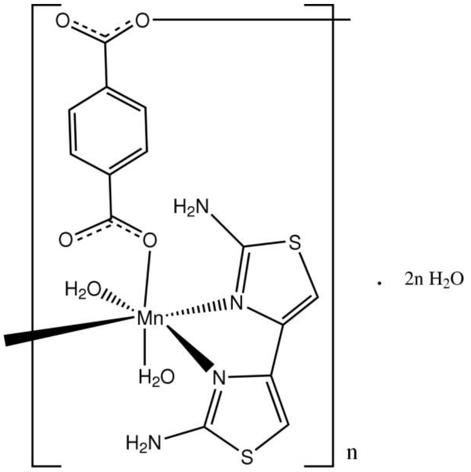
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.034
wR factor = 0.082
Data-to-parameter ratio = 13.5

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

The title Mn^{II} complex, $[Mn(C_8H_4O_4)(C_6H_6N_4S_2)(H_2O)_2]\cdot 2H_2O$, assumes a distorted octahedral coordination geometry formed by 2,2′-diamino-4,4′-bithiazole (DABT), terephthalate dianions and water molecules. The terephthalate dianions, each located on an inversion center, bridge Mn^{II} ions, forming polymeric complex chains. Additionally, π–π stacking is observed between parallel bithiazole ligands.

Comment

Transition metal complexes of diaminobithiazole (DABT) have shown potential application in some fields, for example, a Co^{II} complex and a Ni$_{II}$ complex with the DABT ligand have been found to be effective inhibitors of DNA synthesis of the tumor cells (Waring, 1981; Fisher *et al.*, 1985). As part of ongoing investigations on metal complexes incorporating the DABT ligand (Liu *et al.*, 2001), the title Mn^{II} complex, (I), has been prepared in the laboratory and its X-ray crystallographic structure is reported here.



(I)

The structure of (I) is shown in Fig. 1. The Mn^{II} complex assumes a distorted octahedral coordination (Table 1), formed by a DABT ligand, two terephthalate dianions and two water molecules. The terephthalate dianions, each located on an inversion center, bridge Mn^{II} ions, forming polymeric complex chains (Fig. 1).

The two thiazole rings of the DABT ligand are coplanar, the maximum atomic deviation from the mean plane being 0.0379 (14) Å (for S1). The dihedral angle between the two thiazole planes is 2.60 (10)°, which agrees with 4.57 (7)° found in [Mn(DABT)(oxydiacetate)] (Luo *et al.*, 2004), but different from 20.02 (8)° in [Ni(DABT)(iminodiacetate)] (Liu & Xu, 2005).

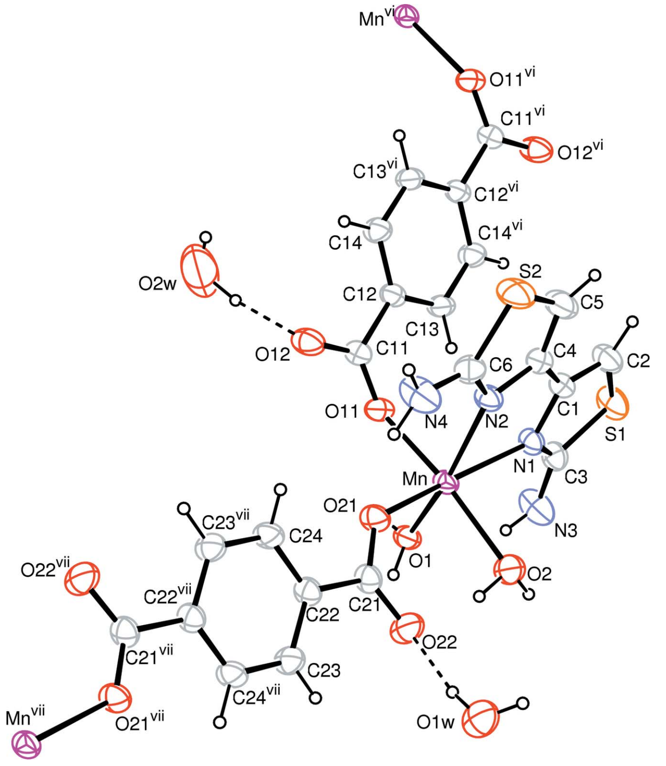


Figure 1
Part of the polymeric structure of (I), shown with 40% probability displacement ellipsoids (arbitrary spheres for H atoms). Dashed lines indicate hydrogen bonds. [Symmetry codes: (vi) $1 - x, 1 - y, 1 - z$; (vii) $2 - x, 3 - y, 1 - z$.]

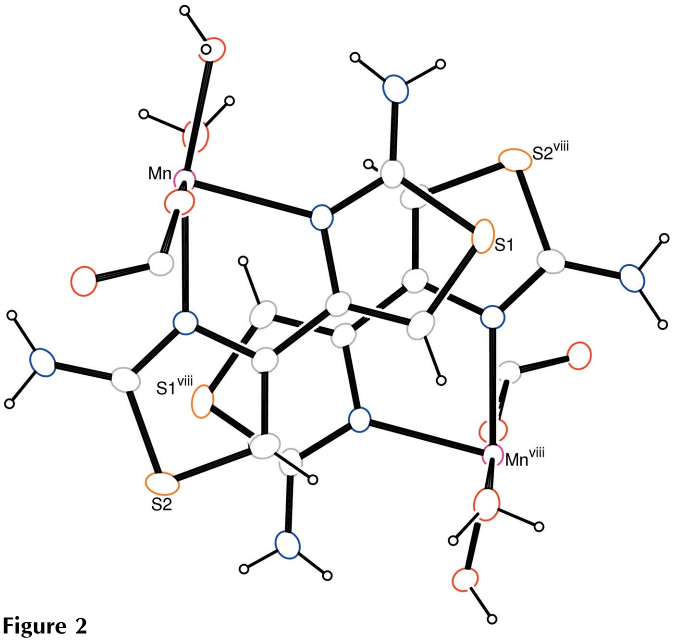


Figure 2
Partially overlapped arrangement of DABT ligands, showing π–π stacking [symmetry code: (viii) $1 - x, 1 - y, -z$].

A partially overlapped arrangement of the parallel thiazole rings is observed (Fig. 2). The face-to-face separation between mean planes of the S1-bithiazole and S1^{viii}-bithiazole ligands is 3.319 (7) Å [symmetry code: (viii) $1 - x, 1 - y, -z$], suggesting the existence of π–π stacking.

An extensive N—H···O and O—H···O hydrogen-bonding network is observed (Table 2), which stabilizes the crystal structure.

Experimental

An aqueous solution (20 ml) containing DABT (0.20 g, 1 mmol) and $MnCl_2\cdot 2H_2O$ (0.16 g, 1 mmol) was mixed with an aqueous solution (10 ml) of terephthalic acid (0.17 g, 2 mmol) and NaOH (0.08 g, 2 mmol). The mixture was refluxed for 6 h. The solution was filtered after cooling to room temperature. Single crystals of (I) were obtained from the filtrate after 3 d.

Crystal data

$[Mn(C_8H_4O_4)(C_6H_6N_4S_2)(H_2O)_2]\cdot 2H_2O$
$M_r = 489.38$
Triclinic, $P\overline{1}$
$a = 10.0666$ (12) Å
$b = 10.2989$ (14) Å
$c = 11.5496$ (15) Å
$\alpha = 111.146$ (13)°
$\beta = 96.060$ (11)°
$\gamma = 111.332$ (14)°
$V = 1000.9$ (3) Å^3
$Z = 2$
$D_x = 1.624$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.92$ mm^{-1}
$T = 295$ (2) K
Prism, yellow
0.25 × 0.18 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.766$, $T_{max} = 0.870$
5305 measured reflections
3550 independent reflections
3085 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 25.2°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.082$
$S = 1.03$
3550 reflections
262 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0346P)^2 + 0.6656P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn—N1	2.2391 (19)	Mn—O2	2.2010 (18)
Mn—N2	2.252 (2)	Mn—O11	2.1470 (17)
Mn—O1	2.2080 (17)	Mn—O21	2.2049 (16)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O1	0.82	2.36	3.061 (4)	143
N3—H3*B*···O1*W*^{i}	0.82	2.14	2.942 (4)	170
N4—H4*A*···O21	0.90	2.34	3.016 (4)	132
N4—H4*B*···O12^{ii}	0.84	2.14	2.959 (4)	166
O1—H1*A*···O21^{iii}	0.84	2.15	2.959 (2)	161
O1—H1*B*···O12^{iii}	0.82	1.93	2.738 (3)	170
O2—H2*A*···O22	0.91	1.75	2.641 (3)	165
O2—H2*B*···O1*W*^{iv}	0.84	2.02	2.839 (3)	167
O1*W*—H1*C*···O22	0.88	1.89	2.762 (3)	170
O1*W*—H1*D*···O2*W*^{v}	0.90	1.83	2.716 (4)	170
O2*W*—H2*C*···O12	0.94	1.88	2.765 (4)	157

Symmetry codes: (i) $x, y - 1, z$; (ii) $-x + 1, -y + 2, -z + 1$; (iii) $-x + 2, -y + 2, -z + 1$; (iv) $-x + 2, -y + 2, -z$; (v) $x, y, z - 1$.

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Amino H atoms and water H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, with $U_{\rm iso}(H) = 1.2U_{\rm eq}(N,O)$. Other H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined as riding, with $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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