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Hexaaquamanganese(II) 5,5′-(1,4-phenylene)-ditetrazolate

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.029
wR factor = 0.081
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.

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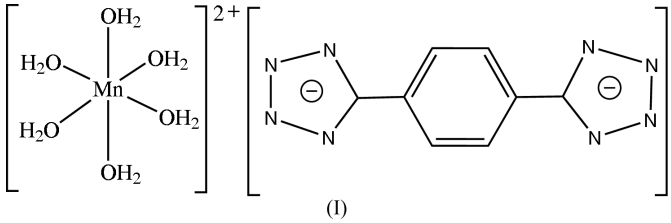
The hydrothermal reaction of manganese chloride tetrahydrate and 5,5′-(1,4-phenylene)bis(1*H*-tetrazole) gave the title compound, $[Mn(H_2O)_6](C_8H_4N_8)$. In the molecule, the Mn^{II} atom is octahedrally coordinated by six water molecules and is located on an inversion center. The centrosymmetric tetrazolate anion remains unligated and links to water *via* hydrogen bonds.

Comment

Much attention has been paid over the last decade to coordination frameworks with channels or pores, because of their potential applications in catalysis (Seo *et al.*, 2000), separation (Uemura *et al.*, 2002), ion exchange (Yaghi & Li, 1995) and gas storage (Rosi *et al.*, 2003). A variety of organic ligands with multifunctional groups have been used to construct the framework. 5,5′-(1,4-Phenylene)bis(1*H*-tetrazole) is one of the most successful ligands used for this purpose. Some examples have been reported (Xiong *et al.*, 2002; Xue *et al.*, 2002; Tao *et al.*, 2004).



(I)

We reported the crystal structure of the coordination polymer of 5,5′-(1,4-phenylene)bis(1*H*-tetrazole) and cadmium(II), which formed a three-dimensional framework with one-dimensional channels (Tao *et al.*, 2004). This paper concerns the reaction of manganese(II) and 5,5′-(1,4-phenyl-

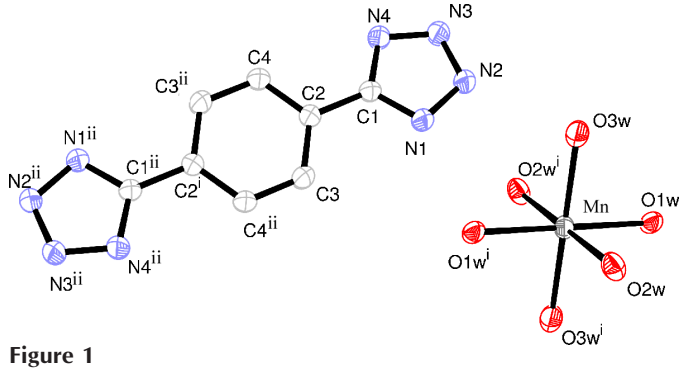


Figure 1
*ORTEP*II plot (Johnson, 1976) of the title compound, with displacement ellipsoids drawn at the 50% probability level [symmetry codes: (i) 1 − *x*, −*y*, 1 − *z*; (ii) 3 − *x*, −*y*, 2 − *z*].

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ene)bis(1*H*-tetrazole), and the crystal structure of the product, (I). However, the results shows that there are no channels in the crystal structure.

In the title compound (Fig. 1), the Mn^{II} ion is coordinated by six water molecules and is located on an inversion center. The coordinated water molecules interact with the uncoordinated centrosymmetric anion *via* hydrogen bonds (Fig. 2, Table 2).

Experimental

Manganese chloride tetrahydrate (0.049 g, 0.25 mmol) and 5,5′-(1,4-phenylene)bis(1*H*-tetrazole) (0.054 g, 0.2 5 mmol) were mixed in water (8 ml). The pH of the solution was adjusted to neutral with sodium hydroxide solution. The solution was transferred into a Teflon-lined stainless steel autoclave and the autoclave was heated to 413 K and maintained at that temperature for 48 h. After cooling to room temperature, crystals suitable for X-ray diffraction were collected.

Crystal data

$[Mn(H_2O)_6](C_8H_4N_8)$
M_r = 375.23
Monoclinic, $P2_1/n$
a = 5.0587 (3) Å
b = 13.4343 (7) Å
c = 11.4989 (6) Å
β = 96.149 (1)°
V = 776.97 (7) Å^3
Z = 2
D_x = 1.604 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4474 reflections
θ = 2.3–28.3°
μ = 0.89 mm^{-1}
T = 296 (2) K
Block, colorless
0.32 × 0.26 × 0.16 mm

Data collection

Bruker SMART APEX 2000 diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.763, T_{max} = 0.870
6205 measured reflections
1674 independent reflections
1599 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 27.0°
$h = -6 \rightarrow 6$
$k = -16 \rightarrow 17$
$l = -13 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.081
S = 1.09
1674 reflections
130 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 0.2423P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O3*W*	2.156 (1)	N3—N4	1.342 (2)
Mn1—O2*W*	2.170 (1)	N4—C1	1.325 (2)
Mn1—O1*W*	2.203 (1)	C1—C2	1.465 (2)
N1—C1	1.328 (2)	C2—C4	1.384 (2)
N1—N2	1.339 (1)	C2—C3	1.390 (2)
N2—N3	1.295 (1)		
O3*W*—Mn1—O2*W*	94.38 (5)	N3—N2—N1	109.2 (1)
O3*W*—Mn1—O1*W*	87.56 (5)	N2—N3—N4	109.5 (1)
O2*W*—Mn1—O1*W*	86.73 (4)	C1—N4—N3	105.0 (1)
C1—N1—N2	105.3 (1)	N4—C1—N1	110.9 (1)

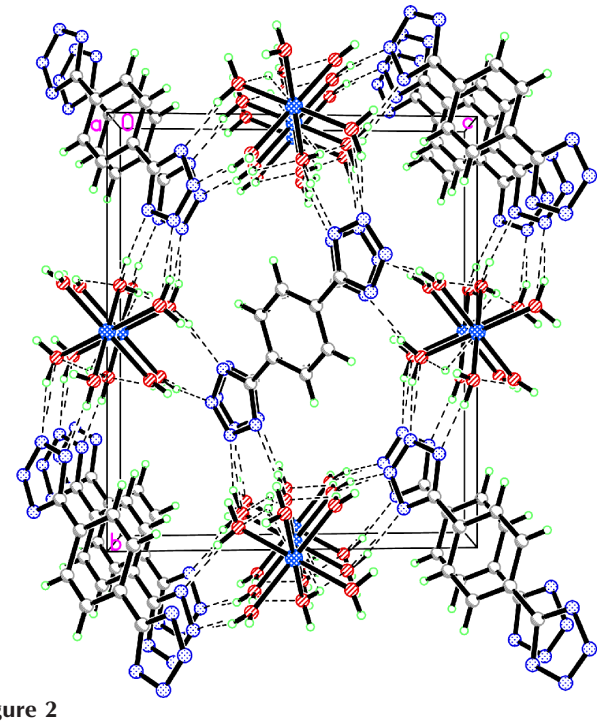

Figure 2
Packing diagram of the title compound, viewed along the *a* axis. Hydrogen bonds are drawn as dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3*W*—H3*WA*···N2	0.838 (9)	1.94 (1)	2.746 (2)	160 (2)
O1*W*—H1*WA*···N1^{i}	0.847 (9)	1.872 (9)	2.706 (1)	168 (2)
O2*W*—H2*WA*···N4^{ii}	0.854 (9)	1.87 (1)	2.720 (2)	172 (2)
O1*W*—H1*WB*···N3^{iii}	0.845 (9)	1.905 (9)	2.721 (2)	162 (1)

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

Water H atoms were initially located in a difference Fourier map and were refined freely with isotropic displacement parameters. The aromatic H atoms were constrained to an ideal geometry, with C—H distances of 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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