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catena-Poly[[diaquamanganese(II)]-di-μ-pyridine-3-sulfonato-κ^2N:O;κ^2O:N]

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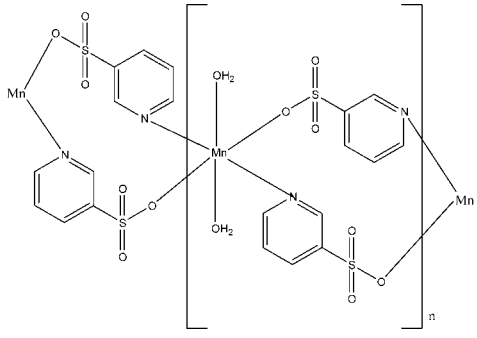
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.027; wR factor = 0.070; data-to-parameter ratio = 14.0.

In the title polymeric complex, $[Mn(C_5H_4NO_3S)_2(H_2O)_2]_n$, the Mn atom is located on a centre of inversion and is coordinated by two O atoms and two N atoms derived from four different pyridine-3-sulfonate ($pySO_3$) ligands, and two O atoms derived from two water molecules in a distorted *trans*-N_2O_4 octahedral geometry. The metal atoms are bridged by the $pySO_3$ ligands to form a one-dimensional chain. The chains are further connected into a three-dimensional architecture *via* hydrogen bonds.

Related literature

For related structures, see: Brodersen *et al.* (1980); Chandrasekhar (1977); Cotton *et al.* (1992*a*,*b*); Mäkinen *et al.*(2001); van der Lee & Barboiu (2004); Walsh & Hathaway (1980). For a description of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$[Mn(C_5H_4NO_3S)_2(H_2O)_2]$
M_r = 407.28
Monoclinic, $P2_1/c$
a = 7.6299 (13) Å
b = 13.201 (2) Å
c = 7.2714 (12) Å
β = 96.516 (3)°
V = 727.7 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.24 mm^{-1}
T = 294 (2) K
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.755, T_{max} = 0.808
4034 measured reflections
1485 independent reflections
1301 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.069
S = 1.06
1485 reflections
106 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4B···O2^{i}	0.89	1.91	2.786 (2)	168
O4—H4A···O1^{ii}	0.89	1.90	2.778 (2)	169

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2137).

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supporting information

Acta Cryst. (2008). E**64**, m765 [doi:10.1107/S1600536808012282]

catena-Poly[[diaquamanganese(II)]-di-μ-pyridine-3-sulfonato-κ^2N:O;κ^2O:N]

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S1. Comment

Structures of complexes or salts based on pyridinium-3-sulfonate are not numerous in the Cambridge Structural Database (CSD; Version 5.25; Allen, 2002). Some six-coordinate metal complexes with pyridine-3-sulfonate ($pySO_3$) ligands that are closely related to the title complex have been reported (Walsh & Hathaway, 1980; Cotton *et al.*, 1992*a*). Other $pySO_3$ complexes are also available (Brodersen *et al.*, 1980; Cotton *et al.*, 1992*b*; Mäkinen *et al.*, 2001; van der Lee & Barboiu, 2004), as well as that of the $pySO_3H$ acid (Chandrasekhar, 1977). There are two structures of the $[M(pySO_3)_2(H_2O)_2]$ type in the CSD. One of them is isostructural with the title compound (Walsh & Hathaway, 1980; Cotton *et al.*, 1992*a*) and the other structure is a two-dimensional coordination polymer (Brodersen *et al.*,1980).

The Mn atom is located on a centre of inversion and is six-coordinated by two N atoms and two O atoms derived from four different $pySO_3$, and two O atoms derived from two water molecules (Fig. 1). The resulting *trans*-N_2O_4 donor set defines a distorted octahedral environment for Mn. The bond angles deviate considerably from 90°; those derived from the bulkier groups deviate by nearly 6°. The Mn—O(water) distance of 2.1681 (15) Å and Mn—O($pySO_3$) distance of 2.1772 (15) Å are in the usual range.The Mn—N distance is also in the usual range for pyridine-like ligands.

The metal ions are bridgeding $pySO_3$ anions to form a chain. In the crystal structure, chains are linked into a 3-D architecture *via* hydrogen bonding interactions (Table 1 & Fig. 2).

S2. Experimental

Pyridinium-3-sulfonate, (1 mmol,159 mg) was dissolved in methanol (A.*R*.,99.9%) (10 ml). To the resulting clear solution was added $MnCl_2.4H_2O$ (0.5 mmol, 98 mg) in methanol (10 ml). After keeping the resulting mixture in air to evaporate about half of the solvent, colourless blocks of the title compound were deposited. The crystals were isolated and washed with alcohol three times (yield 82%). Analysis found (%): C 29.38, H 2.90, N 6.89, S 15.80; $C_{10}H_{12}MnN_2O_8S_2$ requires (%): C 29.47, H 2.94, N 6.87, S 15.71.

S3. Refinement

The H atoms of the water molecules were located in a difference map. The H atoms bonded to C atoms were placed at calculated positions and refined in a riding-model approximation [C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C)]. The O-H distances were standardized to 0.89 Å and the H atoms of the water molecules were refined in a riding-model approximation with U_{iso}(H) = 1.2U_{eq}(O).

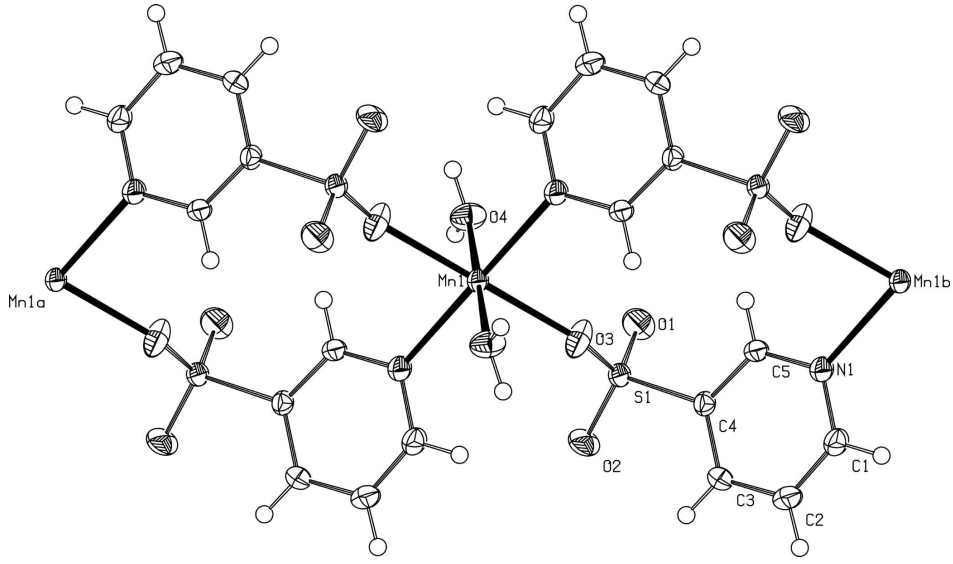

Figure 1

The atom-numbering scheme and 50% probability displacement ellipsoids for the title compound. The Mn atom is located at a center of inversion. H atoms are shown as small spheres of arbitrary radii [symmetry code: (*a*) -1 + *x*,*y*,*z*].

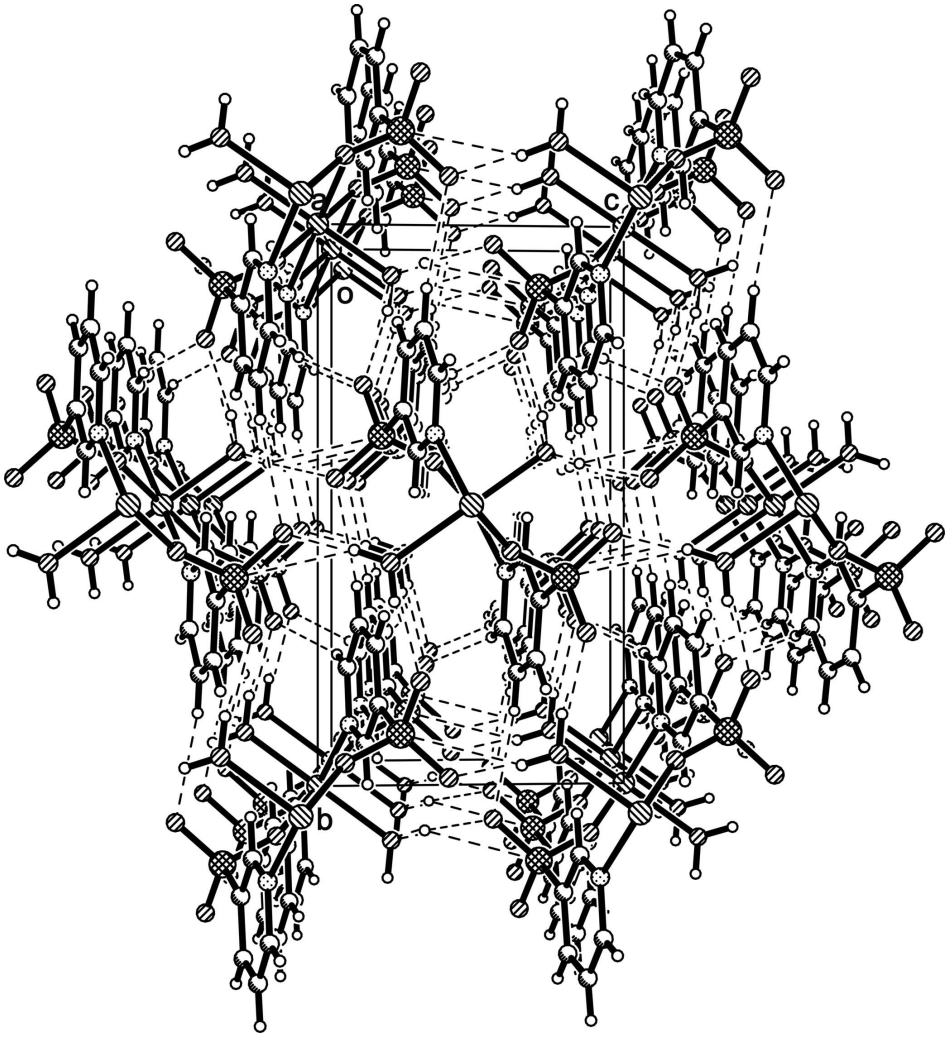

Figure 2

Crystal packing of the title compound viewed approximately down the a-direction showing the hydrogen bonding interactions as dashed lines.

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Crystal data

$[Mn(C_5H_4NO_3S)_2(H_2O)_2]$
$M_r = 407.28$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.6299$ (13) Å
$b = 13.201$ (2) Å
$c = 7.2714$ (12) Å
$\beta = 96.516$ (3)°
$V = 727.7$ (2) Å^3
$Z = 2$
$F(000) = 414$
$D_x = 1.859$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2334 reflections
$\theta = 2.7$–26.4°
$\mu = 1.24$ mm^{-1}
$T = 294$ K
Block, colourless
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.755, T_{max} = 0.808
4034 measured reflections
1485 independent reflections
1301 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 26.4°, θ_{min} = 2.7°
h = −8→9
k = −16→15
l = −9→7

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.069
S = 1.06
1485 reflections
106 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0952P)^2 + 1.5031P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.087 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Mn1	0.0000	1.0000	0.0000	0.01892 (13)
S1	0.72645 (6)	0.87969 (4)	0.28519 (7)	0.01996 (14)
O1	0.7153 (2)	0.95339 (12)	0.4310 (2)	0.0344 (4)
O2	0.8234 (2)	0.78954 (11)	0.3466 (2)	0.0345 (4)
O3	0.7864 (2)	0.92419 (13)	0.1200 (2)	0.0364 (4)
O4	0.0783 (2)	1.09357 (11)	0.2404 (2)	0.0316 (4)
H4A	0.1331	1.0735	0.3492	0.038*
H4B	0.1133	1.1574	0.2295	0.038*
N1	0.2084 (2)	0.88314 (12)	0.1103 (2)	0.0232 (4)
C1	0.1706 (3)	0.78382 (15)	0.1017 (3)	0.0249 (4)
H1	0.0547	0.7645	0.0646	0.030*
C2	0.2946 (3)	0.70884 (16)	0.1449 (3)	0.0296 (5)
H2	0.2627	0.6409	0.1363	0.035*
C3	0.4668 (3)	0.73661 (15)	0.2010 (3)	0.0263 (4)

H3	0.5534	0.6878	0.2303	0.032*
C4	0.5079 (2)	0.83896 (15)	0.2129 (3)	0.0188 (4)
C5	0.3761 (3)	0.90965 (14)	0.1666 (3)	0.0224 (4)
H5	0.4047	0.9781	0.1747	0.027*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0134 (2)	0.0187 (2)	0.0237 (2)	−0.00056 (15)	−0.00157 (16)	0.00122 (16)
S1	0.0146 (2)	0.0193 (2)	0.0250 (3)	0.00040 (17)	−0.00246 (18)	0.00251 (18)
O1	0.0305 (8)	0.0318 (9)	0.0386 (9)	0.0022 (7)	−0.0057 (7)	−0.0107 (7)
O2	0.0252 (8)	0.0247 (8)	0.0499 (10)	0.0067 (6)	−0.0114 (7)	0.0029 (7)
O3	0.0228 (8)	0.0506 (10)	0.0356 (9)	−0.0106 (7)	0.0022 (6)	0.0125 (8)
O4	0.0398 (9)	0.0249 (8)	0.0281 (8)	−0.0042 (7)	−0.0054 (7)	−0.0024 (6)
N1	0.0170 (8)	0.0215 (8)	0.0302 (9)	−0.0009 (7)	−0.0012 (7)	0.0025 (7)
C1	0.0186 (10)	0.0253 (10)	0.0298 (11)	−0.0038 (8)	−0.0014 (8)	0.0006 (9)
C2	0.0281 (12)	0.0184 (10)	0.0416 (13)	−0.0043 (8)	0.0011 (10)	−0.0005 (9)
C3	0.0213 (10)	0.0182 (10)	0.0393 (12)	0.0042 (8)	0.0025 (9)	0.0039 (8)
C4	0.0152 (9)	0.0206 (10)	0.0205 (9)	−0.0006 (7)	0.0009 (7)	0.0013 (7)
C5	0.0186 (10)	0.0156 (9)	0.0322 (11)	−0.0011 (7)	−0.0009 (8)	0.0012 (8)

Geometric parameters (Å, º)

Mn1—O4	2.1681 (15)	N1—C5	1.345 (3)
Mn1—O3^{i}	2.1773 (15)	C1—C2	1.381 (3)
Mn1—N1	2.2937 (16)	C1—H1	0.9300
S1—O2	1.4449 (15)	C2—C3	1.380 (3)
S1—O1	1.4489 (16)	C2—H2	0.9300
S1—O3	1.4570 (16)	C3—C4	1.388 (3)
S1—C4	1.7737 (19)	C3—H3	0.9300
O4—H4A	0.8922	C4—C5	1.385 (3)
O4—H4B	0.8897	C5—H5	0.9300
N1—C1	1.342 (3)		
O4—Mn1—O4^{ii}	180.0	C1—N1—C5	117.40 (17)
O4—Mn1—O3^{i}	95.12 (6)	C1—N1—Mn1	120.26 (13)
O4^{ii}—Mn1—O3^{i}	84.88 (6)	C5—N1—Mn1	121.96 (13)
O3^{iii}—Mn1—O3^{i}	180.0	N1—C1—C2	123.47 (18)
O4—Mn1—N1	89.13 (6)	N1—C1—H1	118.3
O4^{ii}—Mn1—N1	90.87 (6)	C2—C1—H1	118.3
O3^{iii}—Mn1—N1	85.90 (6)	C1—C2—C3	118.80 (19)
O3^{i}—Mn1—N1	94.09 (6)	C1—C2—H2	120.6
N1^{ii}—Mn1—N1	180.00 (6)	C3—C2—H2	120.6
O2—S1—O1	113.41 (10)	C2—C3—C4	118.54 (18)
O2—S1—O3	112.91 (10)	C2—C3—H3	120.7
O1—S1—O3	112.51 (10)	C4—C3—H3	120.7
O2—S1—C4	105.84 (9)	C5—C4—C3	119.22 (18)
O1—S1—C4	106.81 (9)	C5—C4—S1	119.99 (15)

O3—S1—C4	104.50 (9)	C3—C4—S1	120.79 (15)
S1—O3—Mn1^{iv}	146.62 (10)	N1—C5—C4	122.57 (18)
Mn1—O4—H4A	127.1	N1—C5—H5	118.7
Mn1—O4—H4B	121.7	C4—C5—H5	118.7
H4A—O4—H4B	104.2		
O2—S1—O3—Mn1^{iv}	−66.4 (2)	C1—C2—C3—C4	0.4 (3)
O1—S1—O3—Mn1^{iv}	63.6 (2)	C2—C3—C4—C5	−0.6 (3)
C4—S1—O3—Mn1^{iv}	179.06 (19)	C2—C3—C4—S1	179.69 (16)
O4—Mn1—N1—C1	137.80 (16)	O2—S1—C4—C5	172.26 (16)
O4^{ii}—Mn1—N1—C1	−42.20 (16)	O1—S1—C4—C5	51.12 (18)
O3^{iii}—Mn1—N1—C1	−137.26 (16)	O3—S1—C4—C5	−68.31 (18)
O3^{i}—Mn1—N1—C1	42.73 (16)	O2—S1—C4—C3	−8.1 (2)
O4—Mn1—N1—C5	−49.49 (16)	O1—S1—C4—C3	−129.20 (18)
O4^{ii}—Mn1—N1—C5	130.51 (16)	O3—S1—C4—C3	111.38 (18)
O3^{iii}—Mn1—N1—C5	35.44 (16)	C1—N1—C5—C4	0.7 (3)
O3^{i}—Mn1—N1—C5	−144.56 (16)	Mn1—N1—C5—C4	−172.23 (14)
C5—N1—C1—C2	−0.9 (3)	C3—C4—C5—N1	0.1 (3)
Mn1—N1—C1—C2	172.13 (16)	S1—C4—C5—N1	179.77 (16)
N1—C1—C2—C3	0.4 (3)		

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*, −*y*+2, −*z*; (iii) −*x*+1, −*y*+2, −*z*; (iv) *x*+1, *y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*B*···O2^{v}	0.89	1.91	2.786 (2)	168
O4—H4*A*···O1^{vi}	0.89	1.90	2.778 (2)	169

Symmetry codes: (v) −*x*+1, *y*+1/2, −*z*+1/2; (vi) −*x*+1, −*y*+2, −*z*+1.