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Hexaaquamanganese(II) bis[2-(carboxylatomethylsulfanyl)pyridine *N*-oxide]

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Key indicators

Single-crystal X-ray study
T = 303 K
Mean σ(C–C) = 0.003 Å
R factor = 0.024
wR factor = 0.065
Data-to-parameter ratio = 11.3

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

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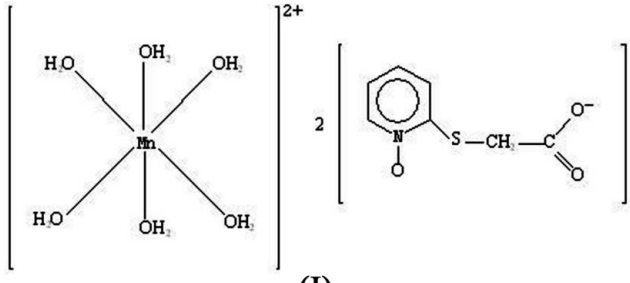
In the title compound, $[Mn(H_2O)_6](C_7H_6NO_3S)_2$, the pyridylsulfanyl *N*-oxide acetate anions have no direct coordination to the Mn^{II} atom. The Mn^{II} atom is octahedrally coordinated by six water molecules and is located on an inversion centre. The cations and anions are linked by O—H···O hydrogen bonds into a three-dimensional network.

Comment

N-Oxides and their derivatives show a broad spectrum of biological activity, such as antifungal, antibacterial, antimicrobial and antibiotic activities (Lobana & Bhatia, 1989). These compounds are also found to be involved in DNA strand scission under physiological conditions (Katsuyuki *et al.*, 1991). In view of the importance of *N*-oxide derivatives, we have previously reported the crystal structure of 2-(acetylsulfanyl)pyridine *N*-oxide (Jebas *et al.*, 2005). As an extension of this work, we report here the crystal structure of the title compound, (I).



(I)

In the title compound (Fig. 1), the Mn^{II} ion is octahedrally coordinated by six water molecules and is located on an inversion centre. The Mn—O distances and O—Mn—O angles are comparable with those reported for other hexaaquamanganese(II) compounds (Wu *et al.*, 1995; Zhang *et al.*, 2005). The C—C, C—O and C—S bond lengths and angles of the anion are normal. The N—O bond length is in good agreement with the mean value of 1.335 (2) Å reported in the literature for pyridine *N*-oxides (Allen *et al.*, 1987). The cation and anion are linked by O—H···O hydrogen bonds, to give a three-dimensional network structure (Table 2).

Experimental

Compound (I) was prepared by heating a mixture of the sodium salt of 2-pyridylsulfanylacetic acid (0.414 g, 2 mmol) and manganese(II) acetate (0.245 g, 1 mmol) in water **(? ml)** at 343 K for 1 h. Single

crystals of (I) were obtained after 7 d by slow cooling of the solution (yield 80%).

Crystal data

$[Mn(H_2O)_6](C_7H_6NO_3S)_2$
M_r = 531.41
Monoclinic, $P2_1/c$
a = 7.413 (1) Å
b = 7.079 (1) Å
c = 20.632 (2) Å
β = 99.530 (7)°
V = 1067.8 (2) Å^3
Z = 2
D_x = 1.653 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.88 mm^{-1}
T = 303 (2) K
Prism, white
0.24 × 0.2 × 0.18 mm

Data collection

Nonius MACH3 diffractometer
ω/θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.810, T_{max} = 0.854
2380 measured reflections
1873 independent reflections
1588 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 25°
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.065
S = 1.04
1873 reflections
166 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 0.3942P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O4	2.1741 (14)	O1—N1	1.340 (2)
Mn1—O5	2.1870 (14)	O2—C7	1.269 (2)
Mn1—O6	2.1894 (14)	O3—C7	1.236 (2)
S1—C5	1.7392 (19)	N1—C1	1.347 (3)
S1—C6	1.8038 (18)	N1—C5	1.362 (2)
O4^i—Mn1—O4	180	O5—Mn1—O6	87.48 (6)
O4—Mn1—O5^i	85.94 (5)	O4—Mn1—O6^i	88.34 (5)
O4—Mn1—O5	94.06 (5)	O5—Mn1—O6^i	92.52 (6)
O5^i—Mn1—O5	180	O6—Mn1—O6^i	180
O4—Mn1—O6	91.66 (5)		

Symmetry code: (i) $-x+1, -y+2, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4B···O1^{ii}	0.84 (1)	1.90 (1)	2.726 (2)	172 (2)
O4—H4B···N1^{ii}	0.84 (1)	2.52 (2)	3.218 (2)	142 (2)
O5—H5B···O2^{iii}	0.85 (1)	1.98 (1)	2.807 (2)	164 (3)
O6—H6A···O2^{iii}	0.84 (1)	2.05 (1)	2.840 (2)	156 (2)
O6—H6B···O1^{iv}	0.84 (1)	1.88 (1)	2.717 (2)	172 (3)
O4—H4A···O3	0.84 (1)	1.86 (1)	2.702 (2)	176 (2)
O5—H5A···O2	0.84 (1)	1.85 (1)	2.683 (2)	170 (3)

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

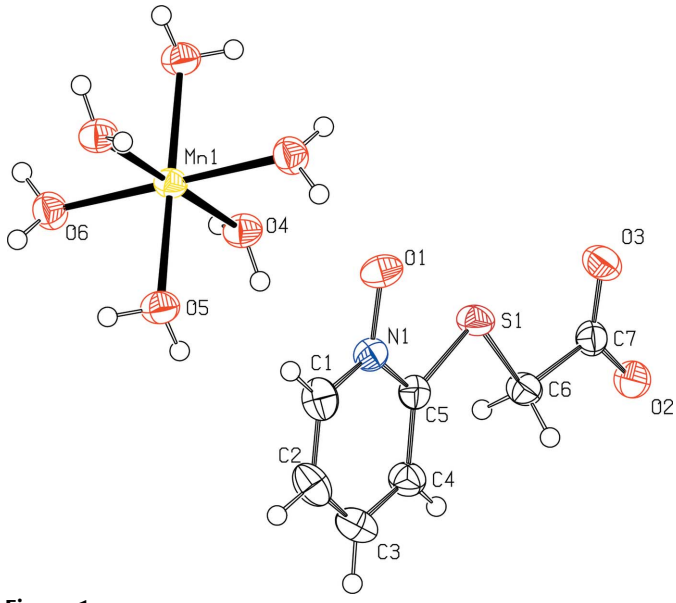


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme for the contents of the asymmetric unit. For clarity, only the independent anion is shown. The other anion and the unlabelled atoms of the cation are generated by the symmetry operation $(1-x, 2-y, 1-z)$.

C-bound H atoms were placed in calculated positions [C—H = 0.93 (aromatic) and 0.97 Å (methylene), and U_{iso}(H) = 1.2U_{eq}(C)] in the riding-model approximation. Water H atoms were located in a difference map and refined with O—H and H···H distance restraints of 0.84 (1) and 1.37 (2) Å, respectively.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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