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Aqua(3,5-dinitrosalicylato-κO)bis(1,10-phenanthroline-$\kappa^2 N,N'$)manganese(II) 3,5-dinitrosalicylate

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In the title compound, $[Mn(C_7H_3N_2O_7)(C_{12}H_8N_2)_2(H_2O)](C_7H_2N_2O_7)$, the Mn^{II} ion is chelated by two phenanthroline ligands, a water molecule and a carboxylate group in an octahedral geometry; the two O atoms involved in bonding are *cis* to each other. The coordinated water molecule links the cation and the carboxylate anion into a linear chain through hydrogen bonds.

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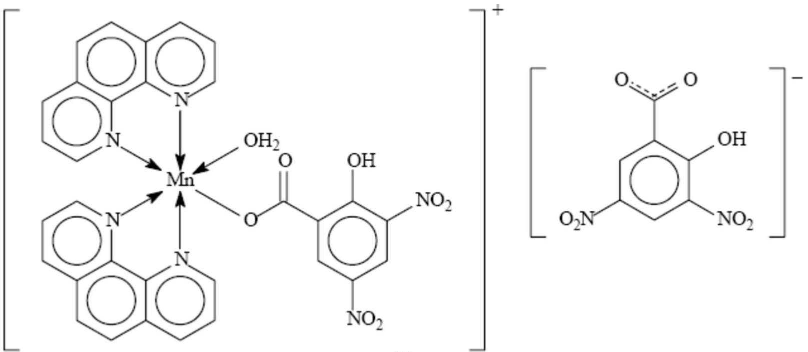
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.047
wR factor = 0.143
Data-to-parameter ratio = 14.9

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

Comment

Whereas a large number of metal derivatives of benzoic acid and its substituted derivatives have been reported, there are few examples of metal derivatives of 3,5-dinitrosalicylic acid, and examples of crystal structure reports are limited to only the silver (Othman *et al.*, 2003), copper (Su & Xu, 2005; Valigura *et al.*, 2004*a*,*b*) and tin (Tian *et al.*, 2005) derivatives. The present manganese derivative, (I), has two chelating 1,10-phenanthroline ligands; probably because of crowding, only one 3,5-dinitrosalicylate group engages in bonding to the metal, whose sixth coordination site is taken up by a water molecule. The hydroxy group of the anion is disordered (Fig. 1). The metal atom shows octahedral coordination (Table 1); the cation and anion interact by hydrogen bonds (Table 2) to form a linear chain motif.



(I)

Experimental

Manganese(II) chloride (0.25 g, 20 mmol) and 1,10-phenanthroline (0.40 g, 20 mmol) were added to a hot aqueous solution (25 ml) of 3,5-dinitrosalicylic acid (0.46 g, 20 mmol). Aqueous sodium hydroxide was added to the solution to a pH of 7 to 8 (approximately 30 mmol). Yellow crystals were isolated from the yellow solution after several days (yield 60%).

Crystal data

$[Mn(C_7H_3N_2O_7)(C_{12}H_8N_2)_2(H_2O)](C_7H_2N_2O_7)$
$M_r = 887.59$
Triclinic, $P\overline{1}$
$a = 11.7446$ (2) Å
$b = 12.4410$ (2) Å
$c = 14.7330$ (2) Å
$\alpha = 66.381$ (1)°
$\beta = 76.477$ (1)°
$\gamma = 87.506$ (1)°
$V = 1914.65$ (5) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.43$ mm^{-1}
$T = 293$ (2) K
$0.30 \times 0.25 \times 0.21$ mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.882$, $T_{max} = 0.915$
30694 measured reflections
8780 independent reflections
5344 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.143$
$S = 1.04$
8780 reflections
589 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.091 (2)	Mn1—N2	2.266 (2)
Mn1—O1*w*	2.144 (2)	Mn1—N3	2.257 (2)
Mn1—N1	2.287 (2)	Mn1—N4	2.275 (2)
O1—Mn1—O1*w*	90.12 (8)	O1*w*—Mn1—N4	88.67 (8)
O1—Mn1—N1	162.60 (8)	N1—Mn1—N2	73.04 (8)
O1—Mn1—N2	91.03 (8)	N1—Mn1—N3	90.47 (8)
O1—Mn1—N3	97.63 (8)	N1—Mn1—N4	97.16 (8)
O1—Mn1—N4	99.90 (7)	N2—Mn1—N3	93.60 (8)
O1*w*—Mn1—N1	86.90 (8)	N2—Mn1—N4	163.84 (8)
O1*w*—Mn1—N2	103.27 (8)	N3—Mn1—N4	73.30 (8)
O1*w*—Mn1—N3	161.32 (8)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O8	0.84 (1)	1.86 (1)	2.701 (3)	176 (2)
O1*w*—H1*w*2···O9^{i}	0.84 (1)	1.84 (1)	2.673 (3)	172 (3)
O14—H14o···O8	0.86 (1)	1.62 (2)	2.435 (4)	158 (4)
O14′—H14′···O9	0.85 (1)	1.63 (6)	2.354 (7)	141 (9)

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

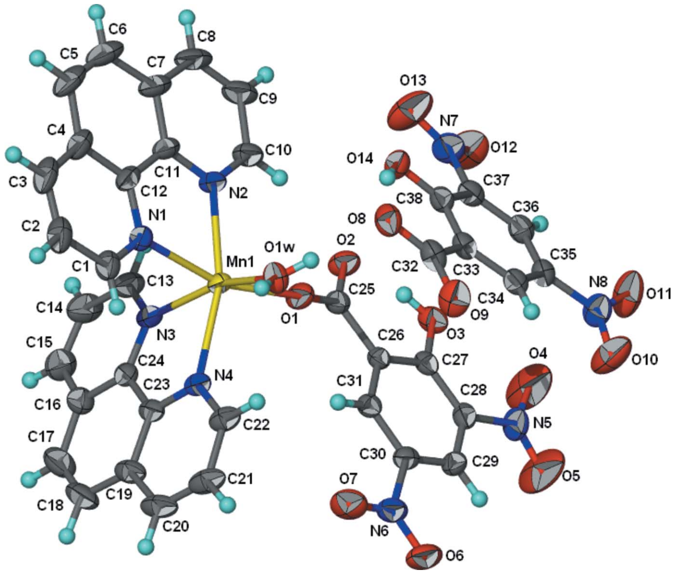


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms as spheres of arbitrary radius. The minor disordered OH component in the anion is not shown.

The hydroxy group of the anion is disordered over two positions; the site occupancy factors refined to 0.622 (5):0.378 (5). Carbon-bound H atoms were placed at calculated positions and were treated as riding on the parent C atoms [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The hydroxy and water H atoms were located in a difference Fourier map, and were refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å; their displacment parameters were freely refined. The larger displacement parameters for atoms O4 and O5 may imply disorder of the N5-nitro group, but this possible disorder was ignored in the refinement.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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