A new manganese(II) complex with the *m*-amino-benzoate anion: [aqua(3-aminobenzoato-κO)-bis(1,10-phenanthroline-$\kappa^2 N,N'$)manganese(II)] 3-aminobenzoate 4.5-hydrate

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Key indicators

Single-crystal X-ray study
$T = 292$ K
Mean σ(C–C) = 0.005 Å
H-atom completeness 95%
Disorder in solvent or counterion
R factor = 0.050
wR factor = 0.143
Data-to-parameter ratio = 16.2

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

In the title compound, $[Mn(C_{12}H_8N_2)_2(C_7H_6NO_2)(H_2O)]\cdot(C_7H_6NO_2)\cdot4.5H_2O$ or $[Mn(phen)_2(L)(H_2O)]L\cdot4.5H_2O$, where H$L$ is *m*-aminobenzoic acid and phen is 1,10-phenanthroline, the central Mn^{II} atom is six-coordinated by four N atoms from two distinct phen ligands, one O atom from a carboxylate ligand and one O atom from a water molecule. The L^- ions and water molecules are linked through an extended network of hydrogen bonds to form a three-dimensional supramolecular structure.

Comment

It is of interest to explore divalent transition metal complexes with biochemical molecules because these complexes show interesting physical–chemical properties, and may find applications in biological systems (Antolini *et al.*, 1982). So far, many studies on the solid-state structures of transition metal complexes with the *o*-aminobenzoate and *p*-aminobenzoate ions have been carried out (Boudreau *et al.*, 1983). However, no study related to the *m*-aminobenzoate ion has been reported. In this paper the crystal structure of a new manganese(II) complex with the *m*-aminobenzoate ligand, (I), is reported.
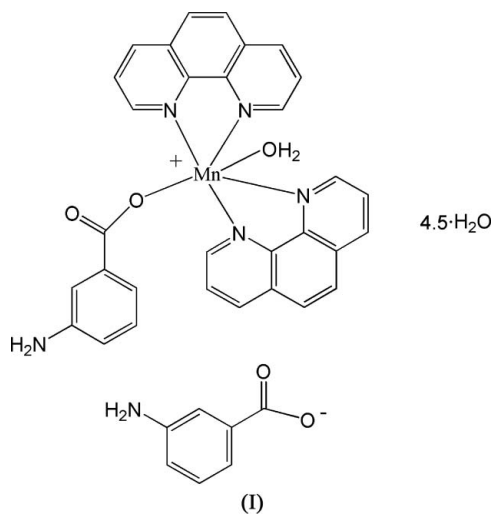
Selected bond lengths and angles for (I) are given in Table 1. Fig. 1 shows the coordination environment of the manganese(II) ion. The manganese(II) ion is six-coordinated by four N atoms from two distinct phen molecules, one carboxylate O atom from an *m*-aminobenzoate anion and one O atom from a water molecule. The Mn—O(carboxylate) distance of 2.114 (2) Å is significantly shorter than the value found in the polymeric compound $[trans-Mn(C_7H_6NO_2)_2(H_2O)_2]_n$ (Li *et al.*,
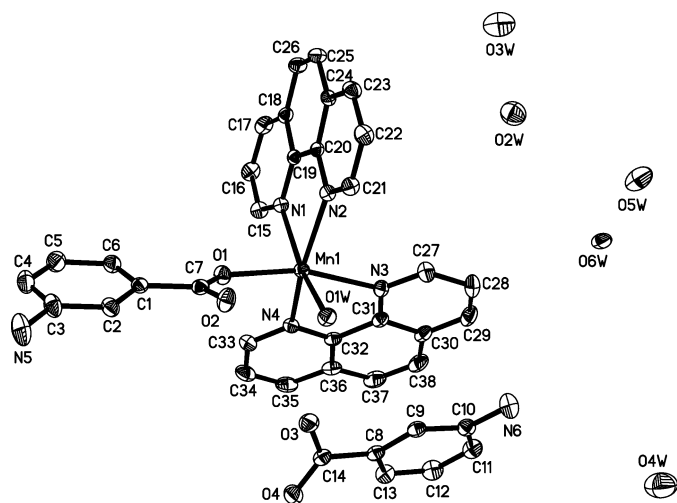
Figure 1
The asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.
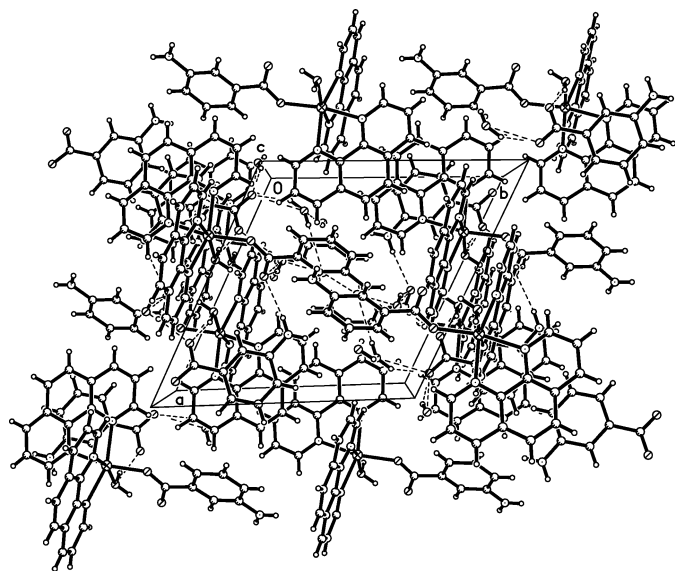

Figure 2
Packing diagram of (I), viewed along the c axis. Intermolecular hydrogen bonds are shown as dashed lines.

2004). In (I), in constras to what is observed in the bis(o-aminobenzoato)copper(II) complex (Lange & Haendler, 1975), the amine group of the m-aminobenzoate ligand is not coordinated to the manganese(II) ion.

In the crystal packing, the ions are linked by an extended network of O—H···O and N—H···O hydrogen bonds (Table 2) to form a three-dimensional supramolecular structure (Fig. 2).

Experimental

m-Aminobenzoic acid (0.274 g, 2 mmol) was added with constant stirring to a suspension of $MnCO_3$ (0.115 g, 1 mmol) in water (10 ml).

1,10-Phenanthroline (0.198 g, 1 mmol) was added to the solution with stirring. Colourless crystals of (I) were obtained from the solution after standing at room temperature for several days (68% yield based on Mn).

Crystal data

$[Mn(C_{12}H_8N_2)_2(C_7H_6NO_2)-$ $(H_2O)](C_7H_6NO_2)\cdot4.5H_2O$	$Z = 2$
$M_r = 786.70$	$D_x = 1.386$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 12.795$ (3) Å	Cell parameters from 13600
$b = 12.800$ (3) Å	reflections
$c = 13.408$ (3) Å	$\theta = 1.8–27.5°$
$\alpha = 102.56$ (3)°	$\mu = 0.42$ mm^{-1}
$\beta = 102.00$ (3)°	$T = 292$ (2) K
$\gamma = 111.91$ (3)°	Block, colourless
$V = 1884.5$ (11) Å^3	$0.42 \times 0.39 \times 0.33$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer	5042 reflections with $I > 2\sigma(I)$
ω scan	$R_{int} = 0.026$
Absorption correction: multi-scan	$\theta_{max} = 27.5°$
(*ABSCOR*; Higashi, 1995)	$h = -16 \rightarrow 16$
$T_{min} = 0.836$, $T_{max} = 0.878$	$k = -15 \rightarrow 16$
13600 measured reflections	$l = -17 \rightarrow 17$
8467 independent reflections	

Refinement

Refinement on F^2	H atoms treated by a mixture of
$R[F^2 > 2\sigma(F^2)] = 0.050$	independent and constrained
$wR(F^2) = 0.143$	refinement
$S = 0.94$	$w = 1/[\sigma^2(F_o^2) + (0.0833P)^2]$
8467 reflections	where $P = (F_o^2 + 2F_c^2)/3$
524 parameters	$(\Delta/\sigma)_{max} < 0.001$
	$\Delta\rho_{max} = 0.86$ e Å^{-3}
	$\Delta\rho_{min} = -0.34$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—Mn1	2.316 (2)	N4—Mn1	2.254 (2)
N2—Mn1	2.270 (2)	O1—Mn1	2.114 (2)
N3—Mn1	2.277 (2)	O1W—Mn1	2.179 (2)
O1—Mn1—O1W	89.66 (8)	N4—Mn1—N3	73.21 (9)
O1—Mn1—N4	94.30 (9)	N2—Mn1—N3	93.98 (9)
O1W—Mn1—N4	106.31 (8)	O1—Mn1—N1	90.77 (8)
O1—Mn1—N2	101.02 (9)	O1W—Mn1—N1	164.20 (8)
O1W—Mn1—N2	91.66 (8)	N4—Mn1—N1	89.40 (8)
N4—Mn1—N2	156.46 (8)	N2—Mn1—N1	72.77 (7)
O1—Mn1—N3	164.11 (8)	N3—Mn1—N1	98.71 (8)
O1W—Mn1—N3	84.67 (8)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—HW12···O2	0.88 (2)	1.88 (2)	2.705 (3)	155 (3)
O1W—HW11···O3	0.90 (2)	1.88 (2)	2.714 (3)	155 (2)
O2W—HW21···O4^i	0.92 (2)	1.94 (2)	2.820 (4)	160 (2)
O3W—HW32···O2W	0.76 (2)	2.29 (3)	2.832 (4)	129 (3)
O4W—HW41···O4^{ii}	0.92 (2)	2.01 (2)	2.852 (4)	152 (4)
N5—H5A···O6W^i	0.86	2.25	2.979 (6)	143
N6—H6A···O2^i	0.86	2.26	3.119 (4)	172
O3W—HW31···O4W^{iii}	0.86 (2)	2.03 (2)	2.882 (5)	174 (3)

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

H atoms attached to C and N atoms were positioned geometrically and refined as riding atoms with C—H = 0.93 Å, N—H = 0.86 Å and $U_{iso}(H) = 1.2U_{eq}(C,N)$. Water H atoms bound to atoms O1W, O2W, O3W and O5W were located in difference Fourier maps. The positions of these atoms were refined freely, with a fixed isotropic displacement parameter (0.054 Å^2). One H atom attached to O4W was also located in a difference Fourier map and refined freely. The remaining H atom bound to atom O4W, and two H atoms bound to O6W were not located in difference Fourier maps and were not included in the model. During the refinement of (I), atom O6W exhibited very large atomic displacement parameters. The occupancy of this atom was refined using a fixed isotropic displacement parameter and converged to 50%. The occupancy was then fixed and anisotropic displacement parameters used for the O atom.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997);

molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL-Plus*.

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