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

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In the title compound, $[Mn(C_7H_5O_3)(C_{12}H_8N_2)_2(H_2O)](C_7H_5O_3)$, the Mn^{II} ion is coordinated by two bidentate phenanthroline molecules, one water molecule and one monodentate 3-hydroxybenzoate (HBA) anion, resulting in a distorted *cis*-MnN_4O_2 octahedral coordination. The uncoordinated HBA anion shows whole-molecule disorder and is hydrogen bonded to the complex cation in the crystal structure by way of O—H···O links.

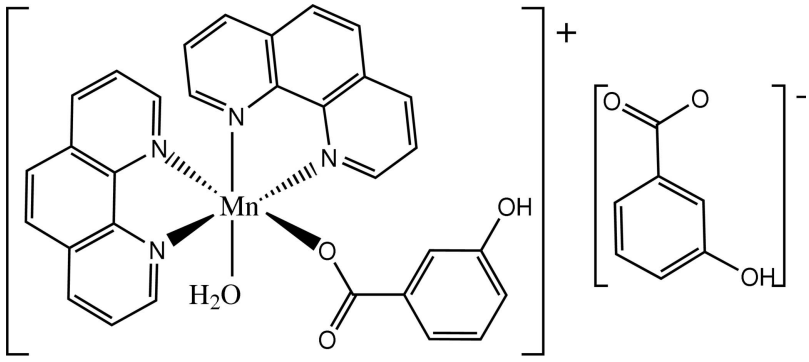
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.042
wR factor = 0.109
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.

Comment

As part of our ongoing investigations of non-covalent interactions in crystals of metal complexes (Li *et al.*, 2005), the title compound, (I), has been prepared and its crystal structure is presented here.



(I)

The crystal structure of (I) consists of Mn^{II} complex cations and uncoordinated 3-hydroxybenzoate (HBA) anions. The Mn^{II} ion is coordinated by two bidentate 1,10-phenanthroline (phen) molecules, one water molecule and one monodentate HBA anion, resulting in a distorted *cis*-MnN_4O_2 octahedral geometry (Fig. 1 and Table 1). This is similar to the situation found in aqua(4-hydroxybenzoato)bis(phenanthroline)-manganese(II) 4-hydroxybenzoate monohydrate (Su *et al.*, 2005). The two phen ligands in (I) are roughly perpendicular to one another, the dihedral angle being 80.65 (5)°. The carboxylate C—O bond lengths of both the coordinated and non-coordinated HBA species suggest localization of the negative charge (Table 1).

Both disordered components of the uncoordinated HBA anion are linked with the complex cation *via* O—H···O hydrogen bonding, between the carboxylate group of HBA and coordinated water molecule of the complex, or between the carboxylate group of HBA and the hydroxyl group of the complex (Table 2).

Experimental

$Mn(CH_3COO)_2{\cdot}4H_2O$ (0.45 g, 1 mmol), sodium 3-hydroxybenzoate (0.16 g, 1 mmol) and phen (0.20 g, 1 mmol) were dissolved in a water/ethanol solution (20 ml, 1:1). The mixture was refluxed for 5 h, and filtered after cooling to room temperature. Single crystals of (I) were obtained after one week.

Crystal data

$[Mn(C_7H_5O_3)(C_{12}H_8N_2)_2(H_2O)](C_7H_5O_3)$
$M_r = 707.58$
Triclinic, $P\overline{1}$
$a = 9.386$ (4) Å
$b = 13.254$ (5) Å
$c = 14.856$ (4) Å
$\alpha = 110.541$ (13)°
$\beta = 91.055$ (13)°
$\gamma = 108.155$ (14)°
$V = 1627.4$ (10) Å^3
$Z = 2$
$D_x = 1.444$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.47$ mm^{-1}
$T = 295$ (3) K
Slab, yellow
0.22 × 0.20 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID CCD diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.896$, $T_{max} = 0.952$
13195 measured reflections
5857 independent reflections
4596 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 25.2°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.109$
$S = 1.03$
5857 reflections
517 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.4519P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn—O1	2.1351 (19)	C31—O32	1.238 (3)
Mn—O31	2.0950 (18)	C31—O31	1.264 (3)
Mn—N1	2.307 (2)	C1*A*—O1*A*	1.219 (7)
Mn—N2	2.253 (2)	C1*A*—O2*A*	1.252 (6)
Mn—N3	2.255 (2)	C1*B*—O1*B*	1.222 (7)
Mn—N4	2.301 (2)	C1*B*—O2*B*	1.255 (5)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O32	0.85	1.83	2.610 (3)	152
O1—H1*B*···O1*B*^{i}	0.86	1.93	2.748 (6)	158
O1—H1*B*···O2*B*	0.86	1.98	2.685 (4)	138
O3*A*—H3*A*···O2*B*^{i}	0.80	1.89	2.592 (6)	146
O3*B*—H3*B*···O2*A*^{ii}	0.91	1.73	2.611 (6)	162
O33—H33*A*···O1*A*^{iii}	0.81	2.17	2.908 (6)	151
O33—H33*A*···O2*A*^{iv}	0.81	1.88	2.613 (5)	148

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

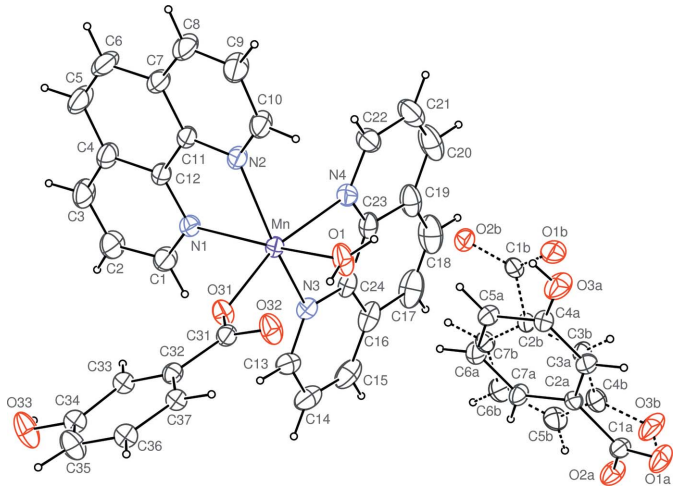


Figure 1
The molecular structure of (I), shown with 25% probability displacement ellipsoids (arbitrary spheres for H atoms). Both disorder components are shown, one of them with dashed bonds.

The uncoordinated HBA anion is disordered over two sites. Occupancies were refined (sum constrained to unity) and converged to 0.507 (6) and 0.493 (6); they were fixed at 0.5 for both components in the final cycles of refinement. The C—C bond distances and C—C—C angles for the disordered benzene rings were fixed at 1.39 Å and 120°, respectively. Water and hydroxyl H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions with $U_{iso}(H) = 1.5U_{eq}(O)$. Other H atoms were placed in calculated positions with C—H = 0.93 Å and refined in riding mode, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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