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A trinuclear manganese(II) complex of 2-acetyl-5-methoxyphenol

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.047
wR factor = 0.115
Data-to-parameter ratio = 13.4

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

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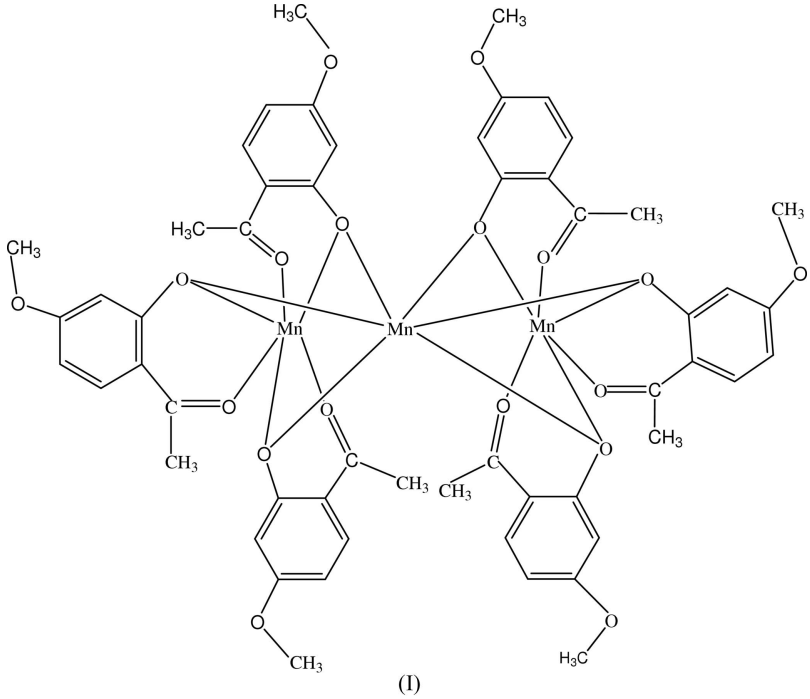
In the title centrosymmetric compound, hexakis(μ-2-acetyl-5-methoxyphenolato)trimanganese(II), $[Mn_3(C_9H_6O_3)_6]$, three Mn^{II} atoms are linearly linked by deprotonated hydroxyl groups of paeonol anions. One Mn atom is located on an inversion center and is coordinated by six hydroxy O atoms, and the Mn atom located on a general position is coordinated by three hydroxy O and three acetyl O atoms. Within the trinuclear molecule, there is a short Mn···Mn separation of 3.0464 (8) Å.

Comment

2-Acetyl-5-methoxyphenol (common name paeonol) is an effective component of many traditional Chinese medicines. Many new metallic complexes of paeonol have been prepared and characterized; however, structural studies of them are rarely reported (Sillanpaa, 1991; Demertzi *et al.*, 2000). Linear trinuclear manganese complexes bridged by acetate anions have been reported previously (Tangoulis *et al.* 1996; Baldwin *et al.* 1995). Recently, we prepared the title Mn^{II} complex, (I), with paeonol ligands and present here its structure.



(I)

The trinuclear molecular structure of (I) is shown in Fig. 1. Three Mn^{II} atoms are linked linearly by deprotonated hydroxyl groups of paeonol anions. Atom Mn1 is located on an inversion center and coordinated by six hydroxy O atoms

with a distorted octahedral geometry. Atom Mn2 is located on a general position and coordinated by three hydroxy O and three acetyl O atoms, with a distorted octahedral geometry (Table 1). Within the trinuclear molecule, there is a short Mn···Mn separation of 3.0464 (8) Å.

Weak C—H···O interactions are observed in the crystal structure (Table 2).

Experimental

A methanol solution (20 ml) of manganese(II) acetate dihydrate (0.184 g, 1.0 mmol) was mixed with a methanol solution (15 ml) of paeonol (0.166 g, 1 mmol). After stirring for 3 h at 320 K, the precipitate was filtered off. Single crystals of (I) were obtained by slow evaporation of the filtrate after 9 d.

Crystal data

$[Mn_3(C_9H_6O_3)_6]$
M_r = 1155.79
Monoclinic, $P2_1/n$
a = 11.967 (2) Å
b = 19.883 (3) Å
c = 12.304 (2) Å
β = 115.740 (2)°
V = 2637.1 (7) Å^3
Z = 2
D_x = 1.456 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.78 mm^{-1}
T = 298 (2) K
Block, yellow
0.19 × 0.18 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.866, T_{max} = 0.912
13782 measured reflections
4647 independent reflections
2690 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.115
S = 1.01
4647 reflections
346 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.032P)^2 + 2.7402P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—O1	2.178 (3)	Mn2—O4	2.172 (3)
Mn1—O4	2.192 (3)	Mn2—O5	2.122 (3)
Mn1—O7	2.162 (3)	Mn2—O7	2.142 (3)
Mn2—O1	2.163 (3)	Mn2—O8	2.128 (3)
Mn2—O2	2.134 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C25—H25···O5^{i}	0.93	2.55	3.396 (5)	151

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

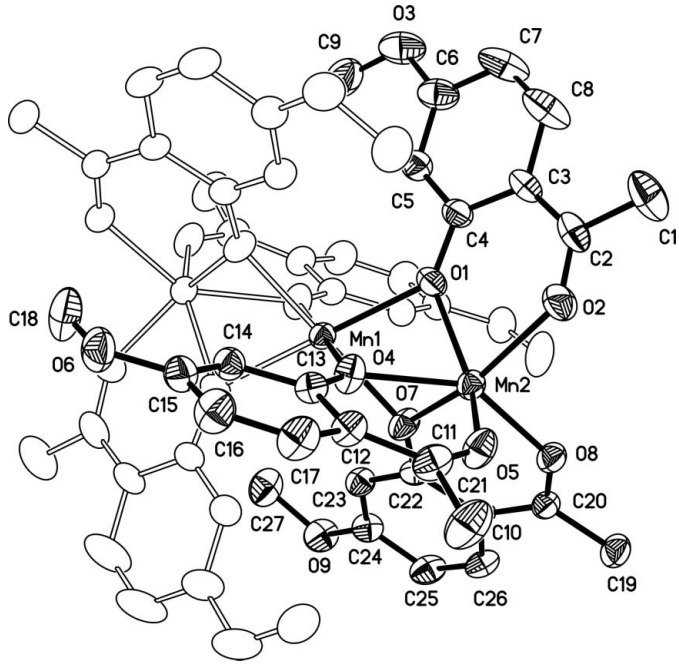


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids, H atoms have been omitted for clarity. Hollow unlabeled atoms are related by the symmetry operator $(1-x, 1-y, 1-z)$.

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and torsion angles were refined to fit the electron density, U_{iso}(H) = 1.5U_{eq}(C). Aromatic H atoms were placed geometrically, with C—H = 0.93 Å, and refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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