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μ-Aqua-bis(μ-4-chlorobenzoato)bis[(4-chlorobenzoato)(1,10-phenanthroline)manganese(**II**)]

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Key indicators

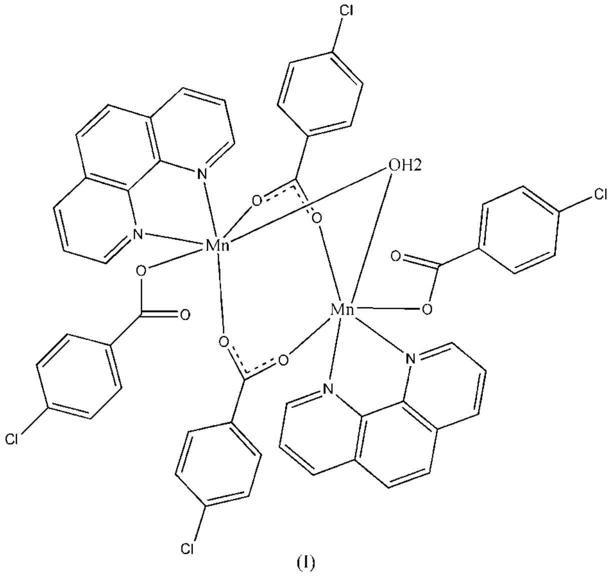
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.045
wR factor = 0.122
Data-to-parameter ratio = 14.9

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

The title complex molecule, $[Mn_2(C_7H_4ClO_2)_4(C_{12}H_8N_2)_2(H_2O)]$, possesses crystallographically imposed C_2 symmetry. Each Mn^{II} atom is coordinated by three carboxyl O atoms from three 4-chlorobenzoate ligands, two N atoms from one 1,10-phenanthroline ligand and one bridging water molecule in a distorted octahedral coordination geometry. The Mn$\cdots$Mn separation is 3.512 (3) Å. Symmetrically related dinuclear molecules form chains parallel to the c axis *via* π–π stacking interactions.

Comment

The design and construction of supramolecular complexes with extended architectures utilizing non-covalent linkages, such as hydrogen-bonding interactions, has been a rapidly developing research area in recent years (Iglesias *et al.*, 2003; Burrows *et al.*, 1997). Hydrogen-bonding interactions between ligands are specific and directional, and have little dependence on the properties of metal ions, playing a critical role in the structures and functions of the products. In this sense, 4-chlorobenzoic acid is an excellent candidate for the construction of supramolecular complexes, since it not only has multiple coordination modes but also can form regular hydrogen bonds by functioning as both hydrogen-bond donor and acceptor (Gu *et al.*, 2004). Recently, we obtained the title novel dinuclear manganese complex, (I), by the reaction of manganese acetate, 4-chlorobenzoic acid and 1,10-phenanthroline in aqueous solution, and its crystal structure is reported here.



(I)

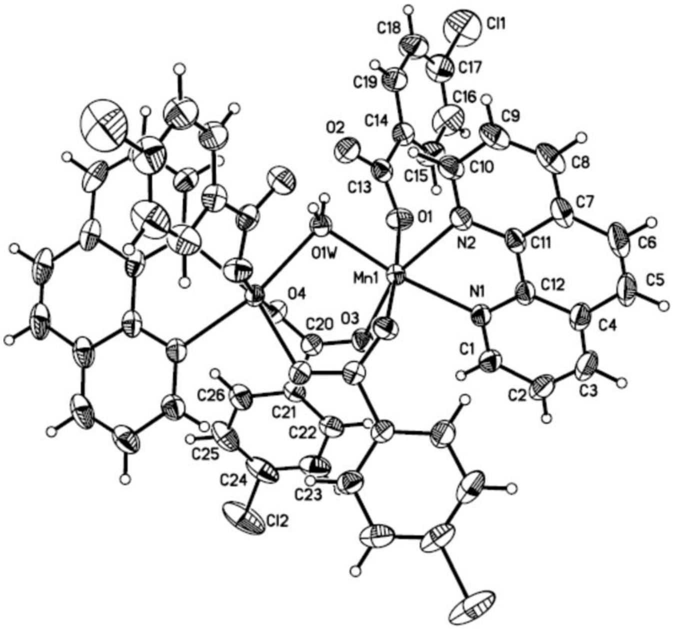


Figure 1
The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Unlabelled atoms are related to the labelled atoms by the symmetry operator ($2 - x$, y, $\frac{3}{2} - z$).

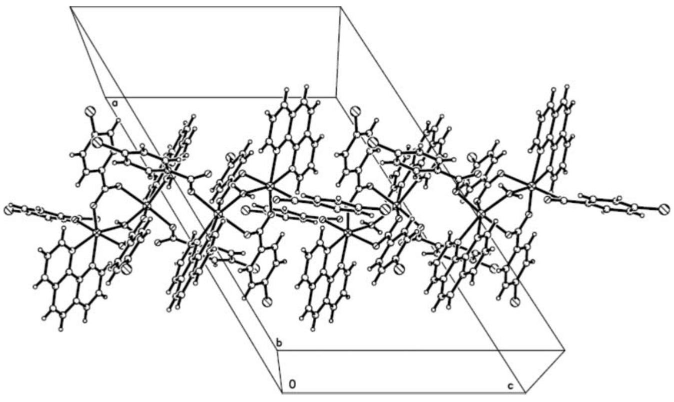


Figure 2
The packing of (I), showing the molecular chain formation along the c axis.

The complex molecule of (I) has a crystallographically imposed twofold rotation symmetry (Fig. 1). Each Mn^{II} centre is coordinated by three carboxyl O atoms from three 4-chlorobenzoic acid ligands, two N atoms from one 1,10-phenanthroline ligand and one μ_2-bridging water molecule in a distorted octahedral coordination geometry (Table 1). The $Mn\cdots Mn$ separation is 3.512 (3) Å. The molecular conformation is stabilized by $O-H\cdots O$ and $C-H\cdots O$ hydrogen bonds (Table 2). In the crystal packing molecules are assembled into chains running parallel to the c axis (Fig. 2) *via* π–π stacking interactions occurring between 4-chlorobenzoic acid and 1,10-phenanthroline ligands of adjacent complexes, with a centroid–centroid distance of 3.627 (3) Å.

Experimental

The title complex was prepared by the addition of a stoichiometric amount of manganese acetate (20 mmol) and 1,10-phenanthroline (20 mmol) to a hot aqueous solution (25 ml) of 4-chlorobenzoic acid (30 mmol). The pH was then adjusted to 7.0-8.0 with NaOH (30 mmol). The resulting solution was filtered, and crystals suitable for X-ray analysis were obtained at room temperature on slow evaporation of the solvent over a period of several days.

Crystal data

$[Mn_2(C_7H_4ClO_2)_4(C_{12}H_8N_2)_2(H_2O)]$
$M_r = 1110.51$
Monoclinic, $C2/c$
$a = 23.4037 (4)$ Å
$b = 15.5866 (3)$ Å
$c = 15.5960 (3)$ Å
$\beta = 121.012 (1)^\circ$
$V = 4875.96 (16)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.80\ mm^{-1}$
$T = 293 (2)$ K
0.30 × 0.25 × 0.18 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.796$, $T_{max} = 0.870$
16907 measured reflections
4789 independent reflections
3220 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.122$
$S = 1.05$
4789 reflections
321 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O3	2.138 (2)	Mn1—N1	2.260 (2)
Mn1—O1	2.148 (2)	Mn1—O1W	2.2624 (18)
Mn1—O4^{i}	2.173 (2)	Mn1—N2	2.295 (2)
O3—Mn1—O1	93.40 (8)	O4^{i}—Mn1—O1W	84.19 (7)
O3—Mn1—O4^{i}	89.04 (8)	N1—Mn1—O1W	162.76 (7)
O1—Mn1—O4^{i}	174.36 (9)	O3—Mn1—N2	160.80 (9)
O3—Mn1—N1	87.70 (9)	O1—Mn1—N2	89.97 (9)
O1—Mn1—N1	98.28 (9)	O4^{i}—Mn1—N2	89.38 (8)
O4^{i}—Mn1—N1	86.90 (8)	N1—Mn1—N2	73.11 (9)
O3—Mn1—O1W	106.84 (7)	O1W—Mn1—N2	92.03 (8)
O1—Mn1—O1W	90.22 (7)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W···O2	0.85	1.74	2.565 (3)	167
C1—H1···O3	0.93	2.56	3.133 (3)	120
C8—H8···O4^{ii}	0.93	2.58	3.450 (5)	156

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

The water H atom was located in a difference density Fourier map, while those bound to C atoms were placed in calculated positions. All H atoms were refined using a riding model with O—H = 0.85 Å, C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(O)$.

m1310 Shen *et al.* • $[Mn_2(C_7H_4ClO_2)_4(C_{12}H_8N_2)_2(H_2O)]$ *Acta Cryst.* (2007). E**63**, m1309–m1311

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Acta Cryst. (2007). E**63**, m1309–m1311 Shen *et al.* • $[Mn_2(C_7H_4ClO_2)_4(C_{12}H_8N_2)_2(H_2O)]$ **m1311**