

Zhao-Peng Deng,^a Shan Gao^a
and Seik Weng Ng^{b*}^aCollege of Chemistry and Materials Science,
Heilongjiang University, Harbin 150080,
People's Republic of China, and ^bDepartment of
Chemistry, University of Malaya, Kuala Lumpur
50603, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

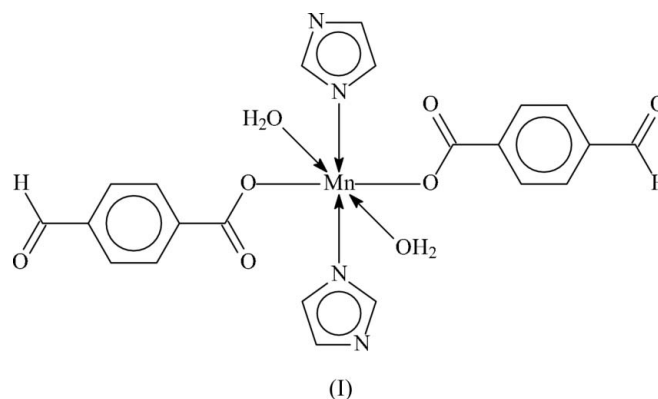
Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
Disorder in main residue
 R factor = 0.033
 wR factor = 0.101
Data-to-parameter ratio = 14.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Diaquabis(4-formylbenzoato- κO)bis(1*H*-
imidazole- κN^3)manganese(II)

The Mn atom in the title compound, $[\text{Mn}(\text{C}_8\text{H}_5\text{O}_3)_2(\text{C}_3\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_2]$, is datively linked to the imidazole heterocycles and water molecules, and covalently linked to the substituted benzoate groups in an all-*trans* octahedral geometry; the Mn atom lies on a center of inversion.

Received 3 August 2006
Accepted 4 August 2006

Comment

Benzoic acid and imidazole are used in the synthesis of a large number of transition metal complexes; the crystal structures of some of these have been reported (Cambridge Structural Database, Version 5.25; Allen, 2002). An example is diaquabis(4-nitrobenzoato)bis(imidazole)manganese, which exists as a centrosymmetric six-coordinate molecule that is hydrogen-bonded into a three-dimensional network motif (Xu & Xu, 2004). However, among the substituted benzoic acids, there is not much information about metal derivatives of 4-formylbenzoic acid in the literature (American Chemical Society, 2006). Although the crystal structure of the acid is known (Haisa *et al.*, 1976), no crystal structure of its metal derivatives has been reported.



The centrosymmetric title complex, (I), has the metal atom in an all-*trans* octahedral geometry; the metal atom is linked covalently to the 4-formylbenzoate group, and datively to the water and imidazole donor ligands (Fig. 1). The coordinated water molecules engage in hydrogen-bonding interactions (Table 2), giving rise to a three-dimensional network motif. The interaction involving the formyl unit is weak, however, and may account for the unit adopting two conformations.

Experimental

Manganese diacetate tetrahydrate (0.122 g, 0.5 mmol) was added to an aqueous solution (10 ml) of 4-formylbenzoic acid (0.15 g, 1 mmol) and imidazole (0.068 g, 1 mmol). The pH value of the mixture was

about 5. The filtered solution was allowed to evaporate at room temperature; colorless prismatic crystals separated after several days. Elemental analysis calculated for $C_{22}H_{22}N_4O_8Mn$: C 50.29, H 4.22, N 10.67%; found: C 50.44, H 3.88, N 10.69%.

Crystal data

$[Mn(C_8H_5O_3)_2(C_3H_4N_2)_2(H_2O)_2]$	$V = 574.3 (4) \text{ \AA}^3$
$M_r = 525.38$	$Z = 1$
Triclinic, $P\bar{1}$	$D_x = 1.519 \text{ Mg m}^{-3}$
$a = 5.644 (2) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 8.141 (4) \text{ \AA}$	$\mu = 0.63 \text{ mm}^{-1}$
$c = 12.940 (5) \text{ \AA}$	$T = 295 (2) \text{ K}$
$\alpha = 75.626 (1)^\circ$	Prism, colorless
$\beta = 86.664 (1)^\circ$	$0.36 \times 0.28 \times 0.15 \text{ mm}$
$\gamma = 86.384 (1)^\circ$	

Data collection

Rigaku RAXIS-RAPID IP diffractometer	5688 measured reflections
ω scans	2616 independent reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	2474 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.662$, $T_{\max} = 0.911$	$R_{\text{int}} = 0.017$
	$\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.061P)^2 + 0.1044P]$
$R[F^2 > 2\sigma(F^2)] = 0.033$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.101$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.15$	$\Delta\rho_{\text{max}} = 0.36 \text{ e \AA}^{-3}$
2616 reflections	$\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$
182 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

Selected geometric parameters (\AA , $^\circ$).

Mn1—O1	2.221 (1)	Mn1—N1	2.230 (2)
Mn1—O1w	2.218 (1)		
O1—Mn1—O1 ⁱ	180	O1w—Mn1—O1w ⁱ	180
O1—Mn1—O1w	88.87 (5)	O1w—Mn1—N1	90.28 (5)
O1—Mn1—O1w ⁱ	91.13 (5)	O1w—Mn1—N1 ⁱ	89.72 (5)
O1—Mn1—N1	93.16 (5)	N1—Mn1—N1 ⁱ	180
O1—Mn1—N1 ⁱ	86.84 (5)		

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

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1w—H1w1 \cdots O1 ⁱⁱ	0.85 (1)	1.97 (1)	2.804 (2)	168 (2)
O1w—H1w2 \cdots O2 ⁱ	0.85 (1)	1.84 (1)	2.667 (2)	168 (3)
N2—H2n \cdots O2 ⁱⁱⁱ	0.85 (1)	2.37 (2)	3.089 (3)	142 (3)
N2—H2n \cdots O3 ^{iv}	0.85 (1)	2.43 (2)	3.044 (3)	129 (3)

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

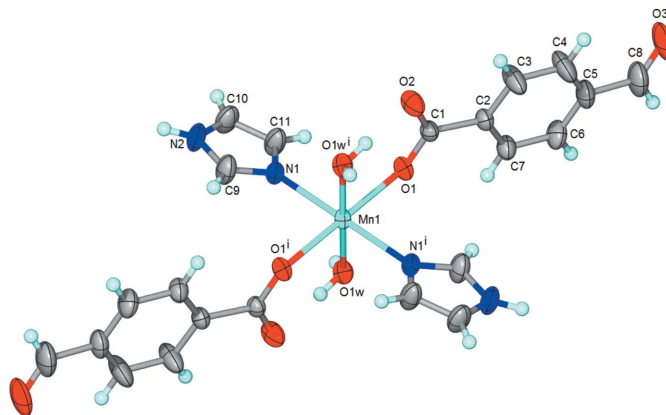


Figure 1

The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. The minor disorder component is not shown. [Symmetry code: (i) $1 - x, 1 - y, 1 - z$.]

The formyl group is disordered over two positions; the occupancies refined to 0.639 (5):0.361 (5). The group was refined as two $CH(=O)$ groups sharing a common C atom; this was necessary for the generation of the riding H atoms. The carbon-bound H atoms were positioned geometrically ($C-H = 0.93 \text{ \AA}$) and were included in the refinement in the riding model approximation, with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$. The amino and water H atoms were located in a difference Fourier map, and were refined with a distance restraint of $N-H = O-H = 0.85 (1) \text{ \AA}$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); 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: *SHELXL97*.

We thank Heilongjiang Province Natural Science Foundation (No. B200501), the Scientific Fund for Remarkable Teachers of Heilongjiang Province (No. 1054 G036) and the University of Malaya for supporting this study.

References

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.
 American Chemical Society (2006). *SciFinder*. American Chemical Society, USA.
 Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
 Haisa, M., Kashino, S., Ikejiri, F., Ohno, T. & Teranishi, K. (1976). *Acta Cryst.* **B32**, 857–860.
 Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
 Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
 Rigaku/MS (2002). *CrystalStructure*. Rigaku/MS Inc., The Woodlands, Texas, USA.
 Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
 Xu, T.-G. & Xu, D.-J. (2004). *Acta Cryst.* **E60**, m1462–m1464.