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Bis(2-methylimidazolium) bis(2-methylimidazole-κN)bis(salicylato-$\kappa^2 O,O'$)manganese(III) bis(methanol-κO)bis(salicylato-$\kappa^2 O,O'$)-manganese(III) methanol disolvate

Lu-Tong Yuan, Zuo-Xiang Wang, An-Yu Zhou, Chun-Yi Liu and Xiao-Yong Chou*

Department of Chemistry & Chemical Engineering, Southeast University, Nanjing 210096, People's Republic of China

Correspondence e-mail: wangzx0908@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.056
wR factor = 0.128
Data-to-parameter ratio = 13.3

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

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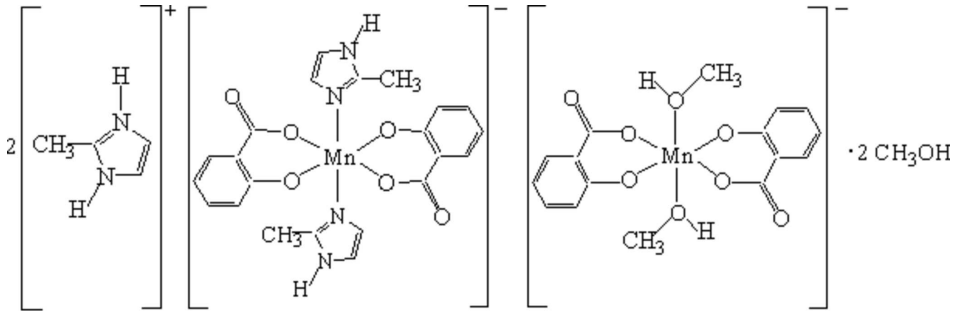
In the title compound, $(C_4H_7N_2)_2[Mn(C_7H_4O_3)_2(C_4H_6N_2)_2][Mn(C_7H_4O_3)_2(CH_4O)_2]\cdot 2CH_4O$, there are two independent Mn^{III} ions, each located on an inversion center. The two Mn^{III} ions assume a distorted octahedral geometry and the complex anions are hydrogen bonded with free methylimidazolium cations and solvent methanol molecules.

Comment

Transition-metal complexes incorporating imidazole or its derivatives have been widely studied because they occur in some biological systems (Bhirud & Srivastava, 1990; Rettig *et al.* 1999; Baca *et al.*, 2003). We report here the crystal structure of the title Mn^{III} complex of methylimidazole, (I).



(I)

The structure of (I) is shown in Fig. 1. In the crystal structure, there are two independent Mn^{III} ions, each located on an inversion center. A measurement of magnetic susceptibility indicates that both Mn1 and Mn2 are trivalent. Mn1 is coordinated by two salicylate dianions and two methylimidazole molecules in a distorted octahedral geometry, and Mn2 is coordinated by two salicylate dianions and two methanol molecules with a similar coordination geometry (Table 1).

Uncoordinated methylimidazolium cations and solvent methanol molecules occur in the crystal structure of (I); they are hydrogen bonded with uncoordinated carboxylate atoms O3 and O6 of the complexes (Table 2).

Experimental

Manganese(II) salicylate (0.70 g, 2.0 mmol) was dissolved in a heated methanol solution (20 ml) of 2-methylimidazole (1.76 g, 20 mmol). The color of the solution changed to brown, indicating the oxidation of Mn^{II} ion. After slow evaporation of the solvent at room temperature, single crystals of (I) were obtained.

Crystal data

$(C_4H_7N_2)_2[Mn(C_7H_4O_3)_2(C_4H_6N_2)_2][Mn(C_7H_4O_3)_2(CH_4O)_2]\cdot 2CH_4O$
$M_r = 1112.90$
Triclinic, $P\overline{1}$
$a = 9.013$ (3) Å
$b = 9.135$ (3) Å
$c = 16.696$ (5) Å
$\alpha = 75.872$ (5)°
$\beta = 85.269$ (5)°
$\gamma = 77.666$ (5)°
$V = 1301.6$ (7) Å^3
$Z = 1$
$D_x = 1.420$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1089 reflections
$\theta = 2.4$–20.6°
$\mu = 0.56$ mm^{-1}
$T = 293$ (2) K
Prism, dark brown
0.28 × 0.24 × 0.22 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{min} = 0.86$, $T_{max} = 0.88$
6480 measured reflections
4497 independent reflections
3402 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 25.0$°
$h = -7 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.128$
$S = 1.08$
4497 reflections
341 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.5222P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—O1	1.863 (2)	Mn2—O4	1.865 (2)
Mn1—O2	1.964 (2)	Mn2—O5	1.912 (2)
Mn1—N1	2.260 (3)	Mn2—O7	2.296 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3^{i}	0.86	2.12	2.949 (5)	163
N3—H3A···O3^{ii}	0.86	2.09	2.947 (4)	177
N4—H4A···O6	0.86	1.98	2.823 (4)	167
O7—H7A···O8^{iii}	0.85	1.96	2.636 (4)	136
O8—H8B···O6	0.85	1.92	2.685 (3)	149

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

Hydroxy H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, with $U_{iso}(H) = 1.2U_{eq}(O)$. Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, the torsion angles refined to fit the electron density, and $U_{iso}(H) = 1.5U_{eq}(C)$. Other H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

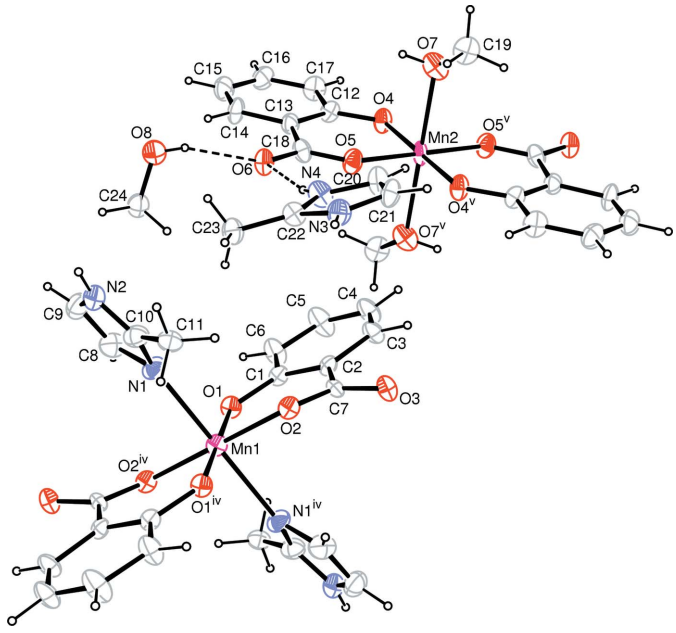


Figure 1
The structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms) [symmetry codes: (iv) $-x, 2-y, -z$; (v) $1-x, 2-y, 1-z$]. Dashed lines indicate hydrogen bonds.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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