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Tetraaquabis[4-(imidazol-1-yl-κN^3)-benzoato]manganese(II)

Lei Zhu,[a] Dabin Wang[b] and Hongyan Xu[b]*

[a]Wuhan Institute of Technology, School of Chemical Engineering and Pharmacy, Hubei 430073, People's Republic of China, and [b]Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, People's Republic of China
Correspondence e-mail: hongyan@fjirsm.ac.cn

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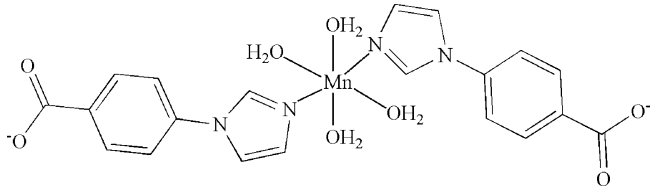
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.113; data-to-parameter ratio = 12.5.

In the title compound, $[Mn(C_{10}H_7N_2O_2)_2(H_2O)_4]$, the Mn^{II} atom, lying on an inversion center, has an octahedral environment with four coordinated water molecules in the equatorial plane and two N atoms from two 4-(imidazol-1-yl)-benzoate ligands at the axial sites. The complex molecules are connected into a three-dimensional network by extensive hydrogen bonds between the water molecules and the carboxylate O atoms.

Related literature

For the good coordination ability and diverse coordination modes of ligands containing imidazole and carboxylate groups, see: Fan *et al.* (2004); Sun *et al.* (2005). For the construction of metal–organic frameworks using ligands based on imidazolyl and carboxylate groups as building blocks, see: Carlucci *et al.* (2008); Zhang *et al.* (2007).



Experimental

Crystal data

$[Mn(C_{10}H_7N_2O_2)_2(H_2O)_4]$
M_r = 501.36
Monoclinic, $P2_1/c$
a = 12.278 (12) Å
b = 11.026 (11) Å
c = 7.978 (7) Å
β = 96.91 (2)°
V = 1072.2 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.67 mm^{-1}
T = 293 K
0.28 × 0.14 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.536, T_{max} = 1.000
7972 measured reflections
2444 independent reflections
2131 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.113
S = 0.91
2444 reflections
195 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H13···O1^{i}	0.85 (2)	2.02 (2)	2.837 (3)	161 (2)
O3—H14···O2^{ii}	0.79 (3)	1.90 (3)	2.688 (3)	179 (2)
O4—H11···O1^{iii}	0.90 (2)	1.82 (2)	2.702 (3)	168 (2)
O4—H12···O1^{i}	0.87 (2)	1.86 (2)	2.694 (3)	158.9 (19)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2292).

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supporting information

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S1. Comment

Over past few years, considerable effort was paied in the study of metal-organic frameworks (MOFs) owing to their intriguing structural diversity and potential application in adsorption, molecular recognition, catalysis and maganetism. The field of molecular magnets has attracted great interest from different horizons for many years. In this context, the ligand containing imidazole and carboxylate groups is of special interest due to its good coordination ability and diverse coordination modes (Fan *et al.*, 2004; Sun *et al.*, 2005). However, the reports of ligands based on imidazole and carboxylate groups as building blocks for the construction of MOFs (Carlucci *et al.*, 2008; Zhang *et al.*, 2007) are still rare. In this paper, we report the synthesis and structural characterzation of the title compound.

As shown in Fig. 1, the molecular structure of the title compound is a momonuclear Mn^{II} complex and the dihedral angle between the imidazolyl ring and the benzene ring of the 4-(imidazol-1-yl)benzoate is 6.3 (2)°. The Mn^{II} ion is coordinated by four water molecules and two N atoms from two different 4-(imidazol-1-yl)benzoate ligands, forming a distorted octahedral coordination environment. The Mn—N and Mn—O bond distances are 2.238 (2) Å and 2.149 (2) and 2.189 (3) Å, respectively. The related hydrogen-bonding geometry is given in Table 1. A l l values involved with hydrogen bonds fall in a normal range. The intermolecular O—H···O hydrogen-bonding interactions between the coordinated water molecules and carboxylate O atoms of 4-(imidazol-1-yl)benzoate ligands lead to the formation of a three-dimensional network structure as shown in Fig. 2.

S2. Experimental

A 10 ml aqueous solution of 4-(imidazole-1-yl)benzoic acid (0.038 g, 0.20 mmol) was slowly added into the manganese(II) perchlorate (0.663 g, 0.30 mmol) solution in methanol (10 ml). The mixed solution was stirred for 20 min and then $HClO_4$ solution was added dropwise with constant stirring until the mixed solution was clear. The resulting solution was filtered and the slow evaporation of filtrate in air gave rise to the desirable products, which were subsequently washed twice with Et_2O (yield 38%).

S3. Refinement

All H atoms were located in a difference Fourier map and refined isotropically.

Figure 1

The molecular structure of the title compound, with the 50% probability displacement ellipsoids. H atoms have been omitted for clarity. [Symmetry code: (i) -x, -y, -z.]

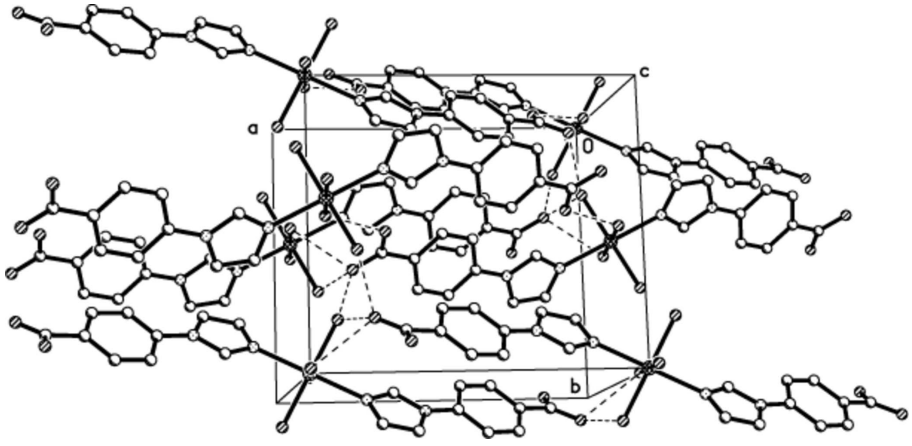

Figure 2

The crystal packing of the title compound, showing O—H···O hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding have been omitted.

Tetraaquabis[4-(imidazol-1-yl-κN^3)benzoato]manganese(II)

Crystal data

$[Mn(C_{10}H_7N_2O_2)_2(H_2O)_4]$
$M_r = 501.36$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.278\ (12)$ Å
$b = 11.026\ (11)$ Å
$c = 7.978\ (7)$ Å
$\beta = 96.91\ (2)°$
$V = 1072.2\ (18)$ Å^3
$Z = 2$
$F(000) = 518$
$D_x = 1.553$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3126 reflections
$\theta = 3.3–27.5°$
$\mu = 0.67$ mm^{-1}
$T = 293$ K
Prism, yellow
0.28 × 0.14 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.536$, $T_{max} = 1.000$
7972 measured reflections
2444 independent reflections
2131 reflections with $I > 2\sigma(I)$

R_{int} = 0.023
θ_{max} = 27.5°, θ_{min} = 2.5°
h = −15→15
k = −14→13
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.113
S = 0.91
2444 reflections
195 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.0000	0.0000	0.0000	0.02675 (15)
O1	−0.85062 (8)	0.13841 (11)	−0.33828 (13)	0.0376 (3)
O2	−0.77609 (10)	0.03929 (15)	−0.53834 (16)	0.0491 (3)
O3	0.02777 (12)	0.01354 (13)	0.27549 (16)	0.0452 (3)
O4	−0.07938 (14)	−0.17041 (13)	0.03407 (19)	0.0636 (5)
N1	−0.16150 (10)	0.09039 (13)	0.01711 (16)	0.0364 (3)
N2	−0.33890 (9)	0.12493 (11)	−0.04316 (14)	0.0289 (3)
C1	−0.25122 (12)	0.06006 (16)	−0.0792 (2)	0.0383 (4)
C2	−0.19202 (15)	0.17902 (19)	0.1215 (3)	0.0523 (5)
C3	−0.30063 (15)	0.20096 (19)	0.0867 (3)	0.0550 (5)
C4	−0.44787 (10)	0.11462 (12)	−0.12551 (16)	0.0259 (3)
C5	−0.52854 (12)	0.19507 (14)	−0.08855 (19)	0.0325 (3)
C6	−0.63403 (12)	0.18533 (14)	−0.1733 (2)	0.0332 (3)
C7	−0.65917 (11)	0.09772 (13)	−0.29617 (17)	0.0265 (3)
C8	−0.57766 (14)	0.01717 (15)	−0.3290 (2)	0.0347 (4)
C9	−0.47314 (14)	0.02432 (16)	−0.2445 (2)	0.0372 (4)
C10	−0.77070 (11)	0.09005 (14)	−0.39869 (17)	0.0301 (3)
H1	−0.254 (3)	0.0002 (18)	−0.158 (4)	0.067 (8)*
H2	−0.139 (2)	0.212 (2)	0.210 (3)	0.068 (7)*
H3	−0.347 (2)	0.254 (2)	0.135 (3)	0.070 (7)*
H5	−0.5108 (14)	0.263 (2)	−0.006 (2)	0.047 (6)*
H6	−0.6944 (15)	0.2366 (18)	−0.149 (2)	0.039 (5)*
H8	−0.5940 (17)	−0.048 (2)	−0.418 (3)	0.052 (5)*
H9	−0.4164 (18)	−0.036 (2)	−0.264 (2)	0.048 (5)*
H11	−0.0941 (19)	−0.239 (2)	−0.025 (3)	0.065 (6)*
H12	−0.1116 (17)	−0.1765 (18)	0.126 (3)	0.047 (5)*
H13	−0.016 (2)	−0.035 (2)	0.316 (3)	0.050 (6)*
H14	0.086 (2)	0.021 (2)	0.330 (3)	0.060 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0172 (2)	0.0347 (2)	0.0279 (2)	−0.00251 (9)	0.00068 (13)	−0.00317 (10)
O1	0.0226 (5)	0.0550 (7)	0.0358 (6)	0.0086 (4)	0.0055 (4)	0.0051 (5)
O2	0.0278 (6)	0.0822 (9)	0.0354 (6)	0.0050 (6)	−0.0040 (5)	−0.0161 (6)
O3	0.0302 (7)	0.0748 (9)	0.0294 (7)	−0.0122 (6)	−0.0018 (5)	−0.0016 (5)
O4	0.0892 (11)	0.0500 (8)	0.0604 (9)	−0.0349 (8)	0.0443 (9)	−0.0225 (7)
N1	0.0238 (6)	0.0475 (8)	0.0367 (6)	0.0026 (5)	−0.0010 (5)	−0.0049 (6)
N2	0.0225 (6)	0.0352 (6)	0.0286 (6)	0.0042 (4)	0.0020 (4)	−0.0011 (5)
C1	0.0229 (7)	0.0500 (10)	0.0413 (8)	0.0063 (6)	0.0008 (6)	−0.0125 (7)
C2	0.0345 (9)	0.0640 (12)	0.0547 (11)	0.0065 (8)	−0.0093 (8)	−0.0253 (9)
C3	0.0340 (9)	0.0664 (12)	0.0613 (12)	0.0119 (8)	−0.0084 (8)	−0.0349 (10)
C4	0.0208 (6)	0.0311 (7)	0.0258 (6)	0.0010 (5)	0.0021 (5)	0.0016 (5)
C5	0.0268 (7)	0.0338 (8)	0.0365 (7)	0.0020 (5)	0.0028 (6)	−0.0087 (6)
C6	0.0240 (6)	0.0356 (8)	0.0404 (8)	0.0066 (5)	0.0062 (6)	−0.0035 (6)
C7	0.0216 (6)	0.0308 (7)	0.0274 (6)	0.0006 (5)	0.0045 (5)	0.0040 (5)
C8	0.0274 (8)	0.0400 (8)	0.0355 (9)	0.0045 (6)	−0.0007 (7)	−0.0098 (6)
C9	0.0268 (8)	0.0413 (8)	0.0425 (9)	0.0105 (6)	0.0004 (7)	−0.0116 (7)
C10	0.0233 (6)	0.0388 (8)	0.0285 (7)	0.0005 (5)	0.0037 (5)	0.0072 (6)

Geometric parameters (Å, º)

Mn1—O4	2.149 (2)	C2—C3	1.351 (3)
Mn1—O3	2.188 (2)	C2—H2	0.97 (2)
Mn1—N1	2.238 (2)	C3—H3	0.93 (3)
O1—C10	1.2623 (19)	C4—C9	1.385 (2)
O2—C10	1.242 (2)	C4—C5	1.387 (2)
O3—H13	0.85 (2)	C5—C6	1.391 (2)
O3—H14	0.79 (3)	C5—H5	1.00 (2)
O4—H11	0.90 (2)	C6—C7	1.385 (2)
O4—H12	0.87 (2)	C6—H6	0.970 (19)
N1—C1	1.308 (2)	C7—C8	1.387 (2)
N1—C2	1.366 (2)	C7—C10	1.511 (2)
N2—C1	1.352 (2)	C8—C9	1.378 (3)
N2—C3	1.371 (2)	C8—H8	1.02 (2)
N2—C4	1.422 (2)	C9—H9	0.99 (2)
C1—H1	0.91 (2)		
O4—Mn1—O4^{i}	180.00 (9)	N2—C1—H1	125 (2)
O4—Mn1—O3	87.18 (6)	C3—C2—N1	109.84 (16)
O4^{i}—Mn1—O3	92.82 (6)	C3—C2—H2	130.1 (14)
O4—Mn1—O3^{i}	92.82 (6)	N1—C2—H2	119.9 (14)
O4^{i}—Mn1—O3^{i}	87.18 (6)	C2—C3—N2	106.62 (16)
O3—Mn1—O3^{i}	180.00 (8)	C2—C3—H3	131.2 (15)
O4—Mn1—N1^{i}	92.12 (9)	N2—C3—H3	122.2 (15)
O4^{i}—Mn1—N1^{i}	87.88 (9)	C9—C4—C5	119.91 (14)
O3—Mn1—N1^{i}	93.41 (6)	C9—C4—N2	119.65 (12)

O3^{i}—Mn1—N1^{i}	86.59 (6)	C5—C4—N2	120.44 (13)
O4—Mn1—N1	87.88 (9)	C4—C5—C6	119.61 (14)
O4^{i}—Mn1—N1	92.12 (9)	C4—C5—H5	120.7 (10)
O3—Mn1—N1	86.59 (6)	C6—C5—H5	119.6 (10)
O3^{i}—Mn1—N1	93.41 (6)	C7—C6—C5	120.87 (13)
N1^{i}—Mn1—N1	180.00 (9)	C7—C6—H6	115.9 (11)
Mn1—O3—H13	108.2 (16)	C5—C6—H6	123.2 (11)
Mn1—O3—H14	125.7 (18)	C6—C7—C8	118.45 (14)
H13—O3—H14	115 (2)	C6—C7—C10	122.20 (13)
Mn1—O4—H11	137.2 (15)	C8—C7—C10	119.32 (14)
Mn1—O4—H12	115.5 (13)	C9—C8—C7	121.45 (15)
H11—O4—H12	107.2 (18)	C9—C8—H8	118.5 (12)
C1—N1—C2	105.52 (14)	C7—C8—H8	120.1 (12)
C1—N1—Mn1	122.68 (12)	C8—C9—C4	119.67 (14)
C2—N1—Mn1	131.77 (11)	C8—C9—H9	121.2 (13)
C1—N2—C3	105.95 (14)	C4—C9—H9	119.1 (13)
C1—N2—C4	126.05 (13)	O2—C10—O1	124.98 (13)
C3—N2—C4	128.00 (13)	O2—C10—C7	117.26 (13)
N1—C1—N2	112.07 (15)	O1—C10—C7	117.73 (14)
N1—C1—H1	123 (2)		

Symmetry code: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H13···O1^{ii}	0.85 (2)	2.02 (2)	2.837 (3)	161 (2)
O3—H14···O2^{iii}	0.79 (3)	1.90 (3)	2.688 (3)	179 (2)
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O4—H12···O1^{ii}	0.87 (2)	1.86 (2)	2.694 (3)	158.9 (19)

Symmetry codes: (ii) −*x*−1, −*y*, −*z*; (iii) *x*+1, *y*, *z*+1; (iv) −*x*−1, *y*−1/2, −*z*−1/2.