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Hexaaquamanganese(II) bis[4-(pyridin-2-ylmethoxy)benzoate] dihydrate

Li-Wei Zhang,[a] Shan Gao[a] and Seik Weng Ng[b,c]*

[a]Key Laboratory of Functional Inorganic Material Chemistry, Ministry of Education, Heilongjiang University, Harbin 150080, People's Republic of China, [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and [c]Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia
Correspondence e-mail: seikweng@um.edu.my

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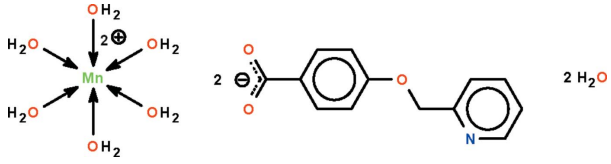
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.060; wR factor = 0.191; data-to-parameter ratio = 17.3.

The Mn^{II} atom in the title salt, $[Mn(H_2O)_6](C_{13}H_{10}NO_3)_2\cdot 2H_2O$, lies on a center of inversion in an octahedron of water molecules. The cations, anions and uncoordinated water molecules are linked by O—H···O and O—H···N hydrogen bonds into a three-dimensional network. The anion is essentially planar, with an r.m.s. deviation of all non-H atoms of 0.068 Å.

Related literature

For the isotypic Co(II) salt, see: Zhang *et al.* (2011).



Experimental

Crystal data

$[Mn(H_2O)_6](C_{13}H_{10}NO_3)_2\cdot 2H_2O$
M_r = 655.51
Triclinic, $P\overline{1}$
a = 7.4895 (18) Å
b = 7.6409 (18) Å
c = 13.791 (3) Å
α = 84.498 (4)°
β = 82.851 (5)°
γ = 72.576 (5)°
V = 745.7 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.51 mm^{-1}
T = 293 K
0.19 × 0.12 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.909, T_{max} = 0.946
7320 measured reflections
3387 independent reflections
1971 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.191
S = 1.07
3387 reflections
196 parameters
18 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H11···O1	0.84	1.94	2.760 (3)	164
O1w—H12···O4w^{i}	0.84	1.83	2.668 (4)	175
O2w—H21···O2	0.85	1.83	2.680 (3)	175
O2w—H22···O2^{ii}	0.85	1.92	2.744 (3)	164
O3w—H31···O1^{iii}	0.84	1.97	2.805 (3)	172
O3w—H32···N1^{iv}	0.85	1.96	2.789 (4)	168
O4w—H41···O2	0.84	2.12	2.888 (4)	151
O4w—H42···O3w^{v}	0.84	2.40	3.165 (4)	151

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5665).

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Acta Cryst. (2011). E**67**, m1520 [doi:10.1107/S1600536811040943]

Hexaaquamanganese(II) bis[4-(pyridin-2-ylmethoxy)benzoate] dihydrate

Li-Wei Zhang, Shan Gao and Seik Weng Ng

S1. Comment

First-row transition metal dications form a plethora of metal dicarboxylates; however, occasionally, no direct metal–carboxylate bond is formed, and the product consists of hexaaquametal cations and carboxylate ions, the anion interacting indirectly in an outer-sphere type of coordination. 4-(Pyridin-2-ylmethoxy)benzoic acid is a commercially available carboxylic acid but there are no reports on its metal carboxylates. The reaction of the deprotonated acid with manganese(II) ions gives the hexaaquamanganese(II) salt (Scheme I, Fig. 1). The Mn^{II} atom in the salt lies on a center-of-inversion in an octahedron of water molecules. The metal atom interacts with the carboxylate ion indirectly, through the coordinated water molecules, in an outer-sphere type of coordination. The cations, anions and lattice water molecules are linked by O···H···O and O–H···N hydrogen bonds into a three-dimensional network (Table 1).

S2. Experimental

Manganese dichloride (1 mmol) was added to an aqueous solution of 4-(pyridin-2-ylmethoxy)benzoic acid (2 mmol) that was earlier been treated with 1*M* sodium hydroxide to a pH of 6. The filtered solution was set aside for several days, after which colorless prismatic crystals separated from solution.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U(C). The water H-atoms were located in a difference Fourier map but were not refined. Their temperature factors were tied by a factor of 1.5 times.

The anisotropic temperature factors of the lattice water O were restrained to be nearly isotropic.

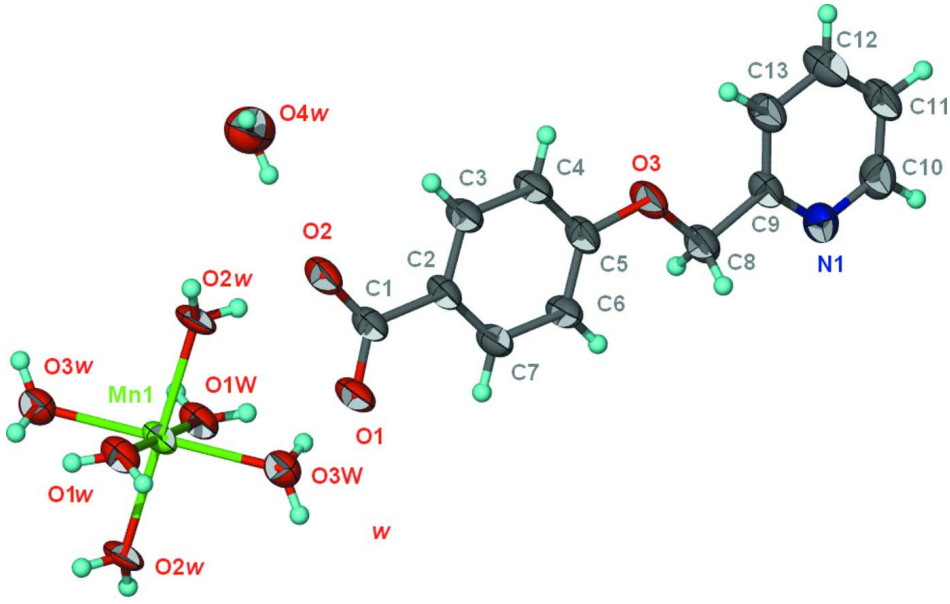

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $Mn(H_2O)_6{\cdot}2(C_{13}H_{10}NO_3){\cdot}2H_2O$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

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c = 13.791 (3) Å
α = 84.498 (4)°
β = 82.851 (5)°
γ = 72.576 (5)°
V = 745.7 (3) Å^3
Z = 1
$F(000)$ = 343
D_x = 1.460 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3613 reflections
θ = 3.1–27.5°
μ = 0.51 mm^{-1}
T = 293 K
Prism, colorless
0.19 × 0.12 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
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ω scans
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7320 measured reflections
3387 independent reflections
1971 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −9→8
k = −9→9
l = −15→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.191
S = 1.07
3387 reflections
196 parameters
18 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0912P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.70$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.5000	0.5000	0.5000	0.0466 (3)
O1	0.4142 (4)	0.8219 (3)	0.26773 (17)	0.0597 (7)
O2	0.3600 (4)	1.0287 (3)	0.37937 (16)	0.0600 (7)
O3	0.2466 (4)	1.5712 (3)	0.00213 (17)	0.0659 (8)
O1w	0.2694 (3)	0.6085 (3)	0.41033 (17)	0.0540 (6)
H11	0.2936	0.6767	0.3620	0.081*
H12	0.1565	0.6540	0.4332	0.081*
O2w	0.4579 (4)	0.7811 (3)	0.52917 (16)	0.0540 (7)
H21	0.4325	0.8561	0.4797	0.081*
H22	0.5051	0.8316	0.5677	0.081*
O3w	0.3151 (4)	0.4446 (3)	0.63159 (16)	0.0571 (7)
H31	0.3960	0.3577	0.6581	0.086*
H32	0.2633	0.5227	0.6736	0.086*
O4w	0.0862 (4)	1.2683 (4)	0.5115 (2)	0.0882 (10)
H41	0.1300	1.1960	0.4663	0.132*
H42	0.1734	1.2742	0.5427	0.132*
N1	0.1726 (4)	1.7360 (4)	−0.2464 (2)	0.0554 (8)
C1	0.3759 (5)	0.9845 (4)	0.2909 (2)	0.0471 (8)
C2	0.3404 (5)	1.1379 (4)	0.2128 (2)	0.0453 (8)
C3	0.3102 (5)	1.3176 (5)	0.2353 (2)	0.0520 (9)
H3	0.3103	1.3441	0.2997	0.062*
C4	0.2800 (6)	1.4580 (5)	0.1630 (2)	0.0562 (10)
H4	0.2595	1.5785	0.1789	0.067*
C5	0.2800 (5)	1.4203 (5)	0.0674 (3)	0.0510 (9)
C6	0.3117 (5)	1.2423 (4)	0.0429 (2)	0.0512 (9)
H6	0.3129	1.2168	−0.0218	0.061*
C7	0.3420 (5)	1.1005 (5)	0.1161 (2)	0.0489 (9)
H7	0.3635	0.9800	0.1000	0.059*
C8	0.2382 (6)	1.5467 (5)	−0.0977 (2)	0.0548 (9)
H8A	0.1441	1.4856	−0.1035	0.066*
H8B	0.3590	1.4720	−0.1258	0.066*
C9	0.1870 (5)	1.7363 (5)	−0.1506 (2)	0.0483 (8)
C10	0.1244 (6)	1.8998 (6)	−0.2957 (3)	0.0645 (11)
H10	0.1140	1.9023	−0.3623	0.077*
C11	0.0898 (6)	2.0632 (5)	−0.2546 (3)	0.0640 (11)
H11A	0.0563	2.1736	−0.2922	0.077*
C12	0.1053 (7)	2.0615 (6)	−0.1567 (3)	0.0705 (12)
H12A	0.0820	2.1706	−0.1261	0.085*

C13	0.1566 (6)	1.8933 (5)	−0.1041 (3)	0.0584 (10)
H13	0.1701	1.8879	−0.0377	0.070*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0650 (6)	0.0290 (4)	0.0490 (5)	−0.0172 (4)	−0.0134 (3)	0.0038 (3)
O1	0.095 (2)	0.0304 (13)	0.0560 (14)	−0.0190 (13)	−0.0203 (13)	0.0039 (10)
O2	0.101 (2)	0.0381 (13)	0.0470 (15)	−0.0260 (14)	−0.0228 (13)	0.0079 (10)
O3	0.117 (2)	0.0380 (14)	0.0449 (14)	−0.0237 (15)	−0.0232 (14)	0.0096 (10)
O1w	0.0678 (17)	0.0374 (13)	0.0593 (14)	−0.0172 (12)	−0.0174 (12)	0.0047 (10)
O2w	0.092 (2)	0.0215 (11)	0.0543 (14)	−0.0192 (12)	−0.0222 (13)	−0.0011 (9)
O3w	0.0719 (18)	0.0417 (14)	0.0531 (14)	−0.0116 (13)	−0.0064 (12)	0.0035 (11)
O4w	0.075 (2)	0.081 (2)	0.108 (2)	−0.0244 (18)	0.0048 (17)	−0.0131 (18)
N1	0.067 (2)	0.0510 (19)	0.0436 (17)	−0.0110 (16)	−0.0098 (14)	0.0072 (13)
C1	0.061 (2)	0.0328 (18)	0.051 (2)	−0.0166 (17)	−0.0157 (16)	0.0043 (14)
C2	0.058 (2)	0.0315 (16)	0.0491 (19)	−0.0164 (16)	−0.0146 (16)	0.0064 (13)
C3	0.079 (3)	0.0356 (18)	0.0445 (19)	−0.0180 (18)	−0.0180 (17)	0.0015 (14)
C4	0.088 (3)	0.0320 (18)	0.051 (2)	−0.0170 (19)	−0.0186 (19)	0.0015 (15)
C5	0.065 (2)	0.0371 (18)	0.051 (2)	−0.0164 (17)	−0.0152 (17)	0.0107 (15)
C6	0.077 (3)	0.0346 (18)	0.0427 (19)	−0.0147 (18)	−0.0149 (17)	−0.0009 (14)
C7	0.068 (2)	0.0324 (17)	0.049 (2)	−0.0159 (17)	−0.0134 (17)	0.0002 (14)
C8	0.070 (3)	0.042 (2)	0.053 (2)	−0.0189 (19)	−0.0115 (18)	0.0070 (16)
C9	0.055 (2)	0.0383 (19)	0.052 (2)	−0.0150 (17)	−0.0111 (16)	0.0062 (15)
C10	0.071 (3)	0.063 (3)	0.050 (2)	−0.008 (2)	−0.0110 (19)	0.0158 (19)
C11	0.082 (3)	0.041 (2)	0.068 (3)	−0.018 (2)	−0.020 (2)	0.0173 (18)
C12	0.096 (3)	0.044 (2)	0.078 (3)	−0.025 (2)	−0.031 (2)	0.0065 (19)
C13	0.086 (3)	0.046 (2)	0.048 (2)	−0.023 (2)	−0.0237 (19)	0.0065 (16)

Geometric parameters (Å, º)

Mn1—O2w^{i}	2.145 (2)	C2—C3	1.383 (5)
Mn1—O2w	2.145 (2)	C2—C7	1.388 (4)
Mn1—O1w	2.163 (2)	C3—C4	1.378 (4)
Mn1—O1w^{i}	2.163 (2)	C3—H3	0.9300
Mn1—O3w	2.229 (2)	C4—C5	1.377 (5)
Mn1—O3w^{i}	2.229 (2)	C4—H4	0.9300
O1—C1	1.252 (4)	C5—C6	1.377 (5)
O2—C1	1.279 (4)	C6—C7	1.394 (4)
O3—C5	1.374 (4)	C6—H6	0.9300
O3—C8	1.418 (4)	C7—H7	0.9300
O1w—H11	0.8420	C8—C9	1.521 (4)
O1w—H12	0.8447	C8—H8A	0.9700
O2w—H21	0.8498	C8—H8B	0.9700
O2w—H22	0.8503	C9—C13	1.360 (5)
O3w—H31	0.8419	C10—C11	1.361 (6)
O3w—H32	0.8451	C10—H10	0.9300
O4w—H41	0.8414	C11—C12	1.368 (5)

O4w—H42	0.8401	C11—H11A	0.9300
N1—C10	1.337 (4)	C12—C13	1.385 (5)
N1—C9	1.339 (4)	C12—H12A	0.9300
C1—C2	1.499 (4)	C13—H13	0.9300
O2w^{i}—Mn1—O2w	180.00 (11)	C2—C3—H3	119.7
O2w^{i}—Mn1—O1w	94.67 (8)	C5—C4—C3	120.2 (3)
O2w—Mn1—O1w	85.33 (8)	C5—C4—H4	119.9
O2w^{i}—Mn1—O1w^{i}	85.33 (8)	C3—C4—H4	119.9
O2w—Mn1—O1w^{i}	94.67 (8)	O3—C5—C4	114.9 (3)
O1w—Mn1—O1w^{i}	180.0	O3—C5—C6	124.7 (3)
O2w^{i}—Mn1—O3w	85.49 (9)	C4—C5—C6	120.4 (3)
O2w—Mn1—O3w	94.51 (9)	C5—C6—C7	119.3 (3)
O1w—Mn1—O3w	93.70 (9)	C5—C6—H6	120.3
O1w^{i}—Mn1—O3w	86.30 (9)	C7—C6—H6	120.3
O2w^{i}—Mn1—O3w^{i}	94.51 (9)	C2—C7—C6	120.5 (3)
O2w—Mn1—O3w^{i}	85.49 (9)	C2—C7—H7	119.7
O1w—Mn1—O3w^{i}	86.30 (9)	C6—C7—H7	119.7
O1w^{i}—Mn1—O3w^{i}	93.70 (9)	O3—C8—C9	107.4 (3)
O3w—Mn1—O3w^{i}	180.0	O3—C8—H8A	110.2
C5—O3—C8	119.0 (3)	C9—C8—H8A	110.2
Mn1—O1w—H11	113.3	O3—C8—H8B	110.2
Mn1—O1w—H12	123.8	C9—C8—H8B	110.2
H11—O1w—H12	108.4	H8A—C8—H8B	108.5
Mn1—O2w—H21	113.9	N1—C9—C13	122.8 (3)
Mn1—O2w—H22	133.0	N1—C9—C8	114.5 (3)
H21—O2w—H22	106.7	C13—C9—C8	122.7 (3)
Mn1—O3w—H31	97.6	N1—C10—C11	124.1 (4)
Mn1—O3w—H32	123.2	N1—C10—H10	117.9
H31—O3w—H32	108.4	C11—C10—H10	117.9
H41—O4w—H42	110.0	C10—C11—C12	118.5 (3)
C10—N1—C9	116.7 (3)	C10—C11—H11A	120.7
O1—C1—O2	123.2 (3)	C12—C11—H11A	120.7
O1—C1—C2	119.5 (3)	C11—C12—C13	118.4 (4)
O2—C1—C2	117.2 (3)	C11—C12—H12A	120.8
C3—C2—C7	119.0 (3)	C13—C12—H12A	120.8
C3—C2—C1	120.8 (3)	C9—C13—C12	119.4 (4)
C7—C2—C1	120.2 (3)	C9—C13—H13	120.3
C4—C3—C2	120.6 (3)	C12—C13—H13	120.3
C4—C3—H3	119.7		
O1—C1—C2—C3	−175.7 (3)	C1—C2—C7—C6	−179.1 (3)
O2—C1—C2—C3	6.2 (5)	C5—C6—C7—C2	0.0 (6)
O1—C1—C2—C7	2.7 (5)	C5—O3—C8—C9	176.3 (3)
O2—C1—C2—C7	−175.4 (3)	C10—N1—C9—C13	−0.5 (6)
C7—C2—C3—C4	0.8 (6)	C10—N1—C9—C8	178.8 (3)
C1—C2—C3—C4	179.2 (4)	O3—C8—C9—N1	−179.6 (3)
C2—C3—C4—C5	−0.2 (6)	O3—C8—C9—C13	−0.3 (5)

C8—O3—C5—C4	−178.1 (3)	C9—N1—C10—C11	−0.1 (6)
C8—O3—C5—C6	1.8 (6)	N1—C10—C11—C12	0.2 (7)
C3—C4—C5—O3	179.4 (4)	C10—C11—C12—C13	0.3 (6)
C3—C4—C5—C6	−0.5 (6)	N1—C9—C13—C12	1.1 (6)
O3—C5—C6—C7	−179.3 (4)	C8—C9—C13—C12	−178.2 (4)
C4—C5—C6—C7	0.6 (6)	C11—C12—C13—C9	−1.0 (7)
C3—C2—C7—C6	−0.7 (6)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H11···O1	0.84	1.94	2.760 (3)	164
O1*w*—H12···O4*w*^{ii}	0.84	1.83	2.668 (4)	175
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O3*w*—H32···N1^{iv}	0.85	1.96	2.789 (4)	168
O4*w*—H41···O2	0.84	2.12	2.888 (4)	151
O4*w*—H42···O3*w*^{v}	0.84	2.40	3.165 (4)	151

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