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catena-Poly[[aqua(pyrazine-2-carboxylato-κ^2N^1,O)manganese(II)]-μ-pyrazine-2-carboxylato-$\kappa^3N^1,O:N^4$]

Yu-Xiang Gao,* Li-Bin Wang, Yan-Ling Niu and Lu-Jiang Hao

Department of Chemistry, Tonghua Teachers' College, Tonghua 134002, People's Republic of China
Correspondence e-mail: yxgao_tonghua@yahoo.com.cn

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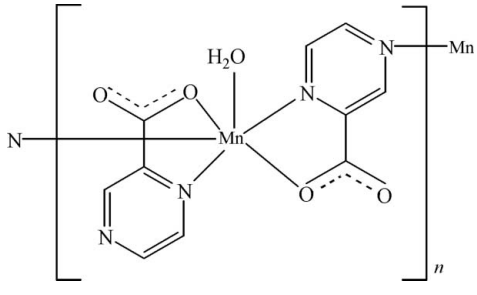
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.039; wR factor = 0.101; data-to-parameter ratio = 14.2.

The title compound, $[Mn(C_5H_3N_2O_2)_2(H_2O)]_n$, prepared by hydrothermal synthesis, is isostructural with its Fe^{II}, Co^{II}, Ni^{II} and Cu^{II} analogues. The asymmetric unit contains two bidendate pyrazine-2-carboxylate anions coordinated to Mn^{II} in the equatorial plane through one N and one O atom. The Mn^{II} atoms are linked into chains by the second N atom of one of the pyrazine-2-carboxylate anions coordinating to an axial site of a neighbouring Mn^{II} atom. The slightly distorted octahedral coordination around Mn^{II} is completed by a water molecule, which forms hydrogen bonds to link the chains into a three-dimensional structure. The investigated crystal was an inversion twin.

Related literature

For the isostructural Fe^{II}, Co^{II}, Ni^{II} and Cu^{II} analogues, see: Hao & Liu (2007); Hao *et al.* (2007); Gao *et al.* (2007*a*,*b*).



Experimental

Crystal data

$[Mn(C_5H_3N_2O_2)_2(H_2O)]$
M_r = 319.14
Orthorhombic, $P2_12_12_1$
a = 7.7220 (10) Å
b = 10.0002 (10) Å
c = 14.8836 (15) Å
V = 1149.33 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.18 mm^{-1}
T = 293 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.891, T_{max} = 0.891
7188 measured reflections
2661 independent reflections
2367 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.101
S = 1.00
2661 reflections
187 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.02 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack (1983), 1086 Friedel pairs
Flack parameter: 0.48 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1W···O4^{i}	0.83 (4)	1.94 (2)	2.742 (4)	162 (6)
O1—H2W···O2^{ii}	0.82 (4)	1.862 (12)	2.681 (4)	171 (5)

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); 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: BI2213).

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supplementary materials

Acta Cryst. (2007). E**63**, m2185 [**doi:10.1107/S1600536807034496**]

catena-Poly[[aqua(pyrazine-2-carboxylato-κ^2N^1,O)manganese(II)]-μ-pyrazine-2-carboxylato-$\kappa^3N^1,O:N^4$]

Y.-X. Gao, L.-B. Wang, Y.-L. Niu and L.-J. Hao

Comment

The title compound, $[Mn(C_5H_3N_2O_2)_2(H_2O)]_n$, is isostructural with its Fe^{II}, Co^{II}, Ni^{II}, and Cu^{II} analogues (Hao & Liu, (2007); Hao, Mu & Liu, (2007); Gao *et al.* (2007*a*); Gao *et al.* (2007*b*)).

The Mn^{II} atom is coordinated in a bidentate fashion by two O and two N atoms from two independent pyrazine-2-carboxylate anions. The distorted octahedral coordiantion is completed by another N atom from a third pyrazine-2-carboxylate ligand, and by the O atom of a water molecule (Figure 1). The Mn—N and Mn—O bond lengths are in the range of 2.094 (3)–2.137 (3) and 2.010 (3)–2.072 (3) Å, respectively.

One pyrazine-2-carboxylate ligand coordinates to a neighbouring Mn^{II} atom *via* its second N atom, leading to a polymeric structure with zigzag chains extending parallel to the *b* axis (Figure 2). Hydrogen bonding between the water molecules stablizes the structure. The refined Flack parameter of 0.48 (3) indicates that the crystal is an inversion twin.

Experimental

All chemicals were used as purchased from Jinan Henghua Sci & Tec Co. Ltd. A mixture of $Mn(CH_3CO_2)_2$ (0.5 mmol), KOH (0.5 mmol), 2-pyrazine carboxylic acid (0.5 mmol), EtOH (8 ml) and H_2O (8 ml) in a 25 ml Teflon-lined stainless steel autoclave was kept at 413 K for 2 d. On cooling to room temperature, colourless crystals were obtained in a yield of 36%. Elemental analysis calculated: C 37.62, H 2.51, N 17.55%; found: C 37.56, H 2.47, N 17.51%.

Refinement

H atoms on C atoms were placed geometrically and refined as riding atoms with C—H = 0.93Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms of the water molecule were located from difference Fourier maps and were refined with distance restraints of O—H = 0.82 (1) Å and H···H = 1.38 (2) Å, and with $U_{iso}(H) = 0.08$ Å^2. The refined Flack parameter (Flack, 1983) from 1086 Friedel pairs is 0.48 (3), indicating that the crystal is an inversion twin.

Figures

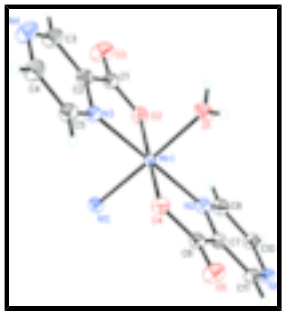

Fig. 1. Asymmetric unit of the title compound expanded to show the complete coordination sphere of Mn^{II}. Displacement ellipsoids are shown at 30% probability for non-H atoms. Symmetry code (I): $1 - x$, $1/2 + y$, $1/2 - z$.

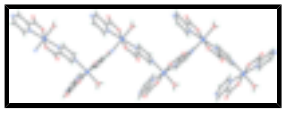

Fig. 2. View of the $[Mn(C_5H_3N_2O_2)_2(H_2O)]_n$ coordination polymer.

catena-Poly[[aqua(pyrazine-2-carboxylato-κ^2N^1,O)manganese(II)]- μ-pyrazine-2-carboxylato-κ^3-κ^2N^1,O:N^4]

Crystal data

$[Mn(C_5H_3N_2O_2)_2(H_2O)]$	F_{000} = 644
M_r = 319.14	D_x = 1.844 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 2661 reflections
a = 7.722 (1) Å	θ = 2.5–28.0º
b = 10.0002 (1) Å	μ = 1.18 mm^{-1}
c = 14.8836 (1) Å	T = 293 (2) K
V = 1149.33 (15) Å^3	Cube, colourless
Z = 4	0.10 × 0.10 × 0.10 mm

Data collection

Bruker APEX II CCD diffractometer	2661 independent reflections
Radiation source: fine-focus sealed tube	2367 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.032
T = 293(2) K	θ_{max} = 28.0º
φ and ω scans	θ_{min} = 2.5º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	h = −9→10
T_{min} = 0.891, T_{max} = 0.891	k = −12→13
7188 measured reflections	l = −15→19

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.039$	$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.7652P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.101$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.00$	$\Delta\rho_{max} = 1.03$ e Å^{-3}
2661 reflections	$\Delta\rho_{min} = -0.33$ e Å^{-3}
187 parameters	Extinction correction: none
3 restraints	Absolute structure: Flack (1983), 1086 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.48 (3)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.1432 (6)	0.5282 (4)	−0.0196 (3)	0.0336 (9)
C2	0.0370 (5)	0.5738 (4)	−0.0409 (3)	0.0328 (9)
C3	0.0750 (6)	0.6650 (4)	−0.1082 (3)	0.0431 (10)
H3	−0.0160	0.7017	−0.1408	0.052*
C4	0.3581 (6)	0.6483 (4)	−0.0792 (3)	0.0432 (10)
H4	0.4724	0.6719	−0.0908	0.052*
C5	0.3240 (6)	0.5575 (4)	−0.0107 (3)	0.0366 (9)
H5	0.4153	0.5233	0.0229	0.044*
C6	0.3050 (5)	0.1913 (4)	0.1834 (3)	0.0277 (8)
C7	0.1282 (5)	0.1459 (4)	0.2115 (2)	0.0270 (7)
C8	−0.1645 (5)	0.1694 (4)	0.2000 (3)	0.0353 (10)
H8	−0.2615	0.2098	0.1749	0.042*
C10	−0.1851 (5)	0.0674 (4)	0.2636 (3)	0.0327 (9)
H10	−0.2964	0.0421	0.2805	0.039*
C11	0.1061 (5)	0.0419 (4)	0.2732 (3)	0.0307 (9)
H11	0.2031	−0.0024	0.2953	0.037*
H1W	0.006 (5)	0.240 (6)	−0.056 (3)	0.080*
H2W	0.156 (5)	0.178 (5)	−0.028 (4)	0.080*
Mn1	0.07321 (6)	0.36583 (5)	0.09074 (3)	0.01617 (13)
N1	−0.0492 (4)	0.0050 (3)	0.3010 (2)	0.0293 (7)

N2	−0.0065 (4)	0.2087 (3)	0.1753 (2)	0.0303 (7)
N3	0.1645 (4)	0.5190 (3)	0.0073 (2)	0.0299 (7)
N4	0.2341 (5)	0.7020 (4)	−0.1282 (3)	0.0505 (10)
O1	0.0814 (5)	0.2346 (3)	−0.01690 (19)	0.0399 (7)
O2	−0.1538 (4)	0.4351 (3)	0.04084 (19)	0.0333 (6)
O3	−0.2617 (4)	0.5807 (4)	−0.0589 (3)	0.0567 (9)
O4	0.3053 (3)	0.2971 (3)	0.13085 (18)	0.0315 (6)
O5	0.4313 (4)	0.1305 (3)	0.20942 (19)	0.0415 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.029 (2)	0.036 (2)	0.036 (2)	−0.0012 (17)	−0.0035 (17)	0.0013 (17)
C2	0.035 (2)	0.033 (2)	0.030 (2)	0.0042 (17)	−0.0003 (16)	−0.0001 (16)
C3	0.033 (2)	0.048 (2)	0.049 (3)	0.002 (2)	−0.005 (2)	0.0146 (18)
C4	0.035 (2)	0.044 (2)	0.051 (3)	−0.002 (2)	0.005 (2)	0.009 (2)
C5	0.032 (2)	0.037 (2)	0.041 (2)	0.0014 (18)	−0.0017 (18)	0.0019 (17)
C6	0.0222 (18)	0.0309 (18)	0.0300 (19)	−0.0004 (15)	−0.0003 (14)	−0.0031 (15)
C7	0.0266 (17)	0.0282 (18)	0.0262 (17)	0.0032 (15)	0.0021 (13)	−0.0009 (16)
C8	0.0233 (19)	0.042 (3)	0.040 (2)	−0.0008 (18)	−0.0011 (17)	0.0003 (18)
C10	0.027 (2)	0.033 (2)	0.038 (2)	−0.0034 (17)	0.0000 (16)	0.0052 (17)
C11	0.027 (2)	0.0339 (19)	0.0308 (19)	0.0019 (16)	0.0003 (16)	0.0025 (16)
Mn1	0.0136 (2)	0.0179 (2)	0.0170 (2)	−0.00008 (19)	0.00074 (19)	0.00062 (19)
N1	0.0295 (17)	0.0290 (15)	0.0293 (15)	−0.0008 (14)	−0.0005 (14)	0.0049 (13)
N2	0.0247 (15)	0.0327 (17)	0.0334 (18)	−0.0010 (14)	0.0014 (14)	−0.0021 (14)
N3	0.0293 (17)	0.0296 (17)	0.0307 (17)	−0.0006 (14)	−0.0006 (14)	0.0019 (13)
N4	0.042 (2)	0.055 (2)	0.055 (2)	−0.007 (2)	0.0056 (19)	0.019 (2)
O1	0.0371 (16)	0.0445 (16)	0.0383 (15)	0.0116 (16)	−0.0078 (14)	−0.0132 (13)
O2	0.0231 (13)	0.0360 (15)	0.0407 (16)	−0.0022 (12)	0.0007 (12)	−0.0003 (13)
O3	0.0314 (17)	0.076 (2)	0.063 (2)	0.0063 (17)	−0.0064 (15)	0.0208 (19)
O4	0.0267 (14)	0.0359 (15)	0.0321 (14)	−0.0014 (12)	0.0022 (11)	0.0018 (12)
O5	0.0258 (13)	0.0494 (16)	0.0492 (16)	0.0051 (17)	−0.0006 (13)	0.0100 (14)

Geometric parameters (Å, °)

C1—O3	1.206 (5)	C8—N2	1.334 (5)
C1—O2	1.297 (5)	C8—C10	1.401 (6)
C1—C2	1.498 (6)	C8—H8	0.930
C2—N3	1.335 (5)	C10—N1	1.341 (5)
C2—C3	1.387 (6)	C10—H10	0.930
C3—N4	1.317 (6)	C11—N1	1.321 (5)
C3—H3	0.930	C11—H11	0.930
C4—N4	1.318 (6)	Mn1—O4	2.010 (3)
C4—C5	1.390 (6)	Mn1—O2	2.026 (3)
C4—H4	0.930	Mn1—O1	2.072 (3)
C5—N3	1.318 (5)	Mn1—N3	2.094 (3)
C5—H5	0.930	Mn1—N2	2.106 (3)
C6—O5	1.213 (5)	Mn1—N1^{i}	2.137 (3)

C6—O4	1.315 (5)	N1—Mn1^{ii}	2.137 (3)
C6—C7	1.498 (5)	O1—H1W	0.83 (4)
C7—N2	1.329 (5)	O1—H2W	0.82 (4)
C7—C11	1.399 (5)		
O3—C1—O2	126.9 (4)	O4—Mn1—O2	175.74 (12)
O3—C1—C2	118.0 (4)	O4—Mn1—O1	89.19 (12)
O2—C1—C2	115.1 (3)	O2—Mn1—O1	87.68 (12)
N3—C2—C3	120.1 (4)	O4—Mn1—N3	97.25 (12)
N3—C2—C1	116.5 (3)	O2—Mn1—N3	79.85 (12)
C3—C2—C1	123.3 (4)	O1—Mn1—N3	89.68 (13)
N4—C3—C2	123.0 (4)	O4—Mn1—N2	80.08 (12)
N4—C3—H3	118.5	O2—Mn1—N2	102.79 (12)
C2—C3—H3	118.5	O1—Mn1—N2	89.91 (13)
N4—C4—C5	122.3 (4)	N3—Mn1—N2	177.31 (14)
N4—C4—H4	118.9	O4—Mn1—N1^{i}	94.36 (12)
C5—C4—H4	118.9	O2—Mn1—N1^{i}	88.78 (12)
N3—C5—C4	121.1 (4)	O1—Mn1—N1^{i}	176.45 (14)
N3—C5—H5	119.4	N3—Mn1—N1^{i}	90.00 (13)
C4—C5—H5	119.4	N2—Mn1—N1^{i}	90.57 (12)
O5—C6—O4	126.3 (4)	C11—N1—C10	116.8 (3)
O5—C6—C7	119.5 (3)	C11—N1—Mn1^{ii}	119.7 (3)
O4—C6—C7	114.3 (3)	C10—N1—Mn1^{ii}	123.2 (3)
N2—C7—C11	121.5 (3)	C7—N2—C8	117.7 (3)
N2—C7—C6	117.2 (3)	C7—N2—Mn1	111.4 (3)
C11—C7—C6	121.3 (3)	C8—N2—Mn1	130.7 (3)
N2—C8—C10	120.3 (4)	C5—N3—C2	117.4 (3)
N2—C8—H8	119.8	C5—N3—Mn1	130.5 (3)
C10—C8—H8	119.8	C2—N3—Mn1	111.7 (3)
N1—C10—C8	122.0 (4)	C3—N4—C4	116.0 (4)
N1—C10—H10	119.0	Mn1—O1—H1W	119 (3)
C8—C10—H10	119.0	Mn1—O1—H2W	128 (3)
N1—C11—C7	121.6 (3)	H1W—O1—H2W	113 (3)
N1—C11—H11	119.2	C1—O2—Mn1	116.4 (3)
C7—C11—H11	119.2	C6—O4—Mn1	116.7 (2)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1W···O4^{iii}	0.83 (4)	1.94 (2)	2.742 (4)	162 (6)
O1—H2W···O2^{iv}	0.82 (4)	1.862 (12)	2.681 (4)	171 (5)

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

Fig. 1

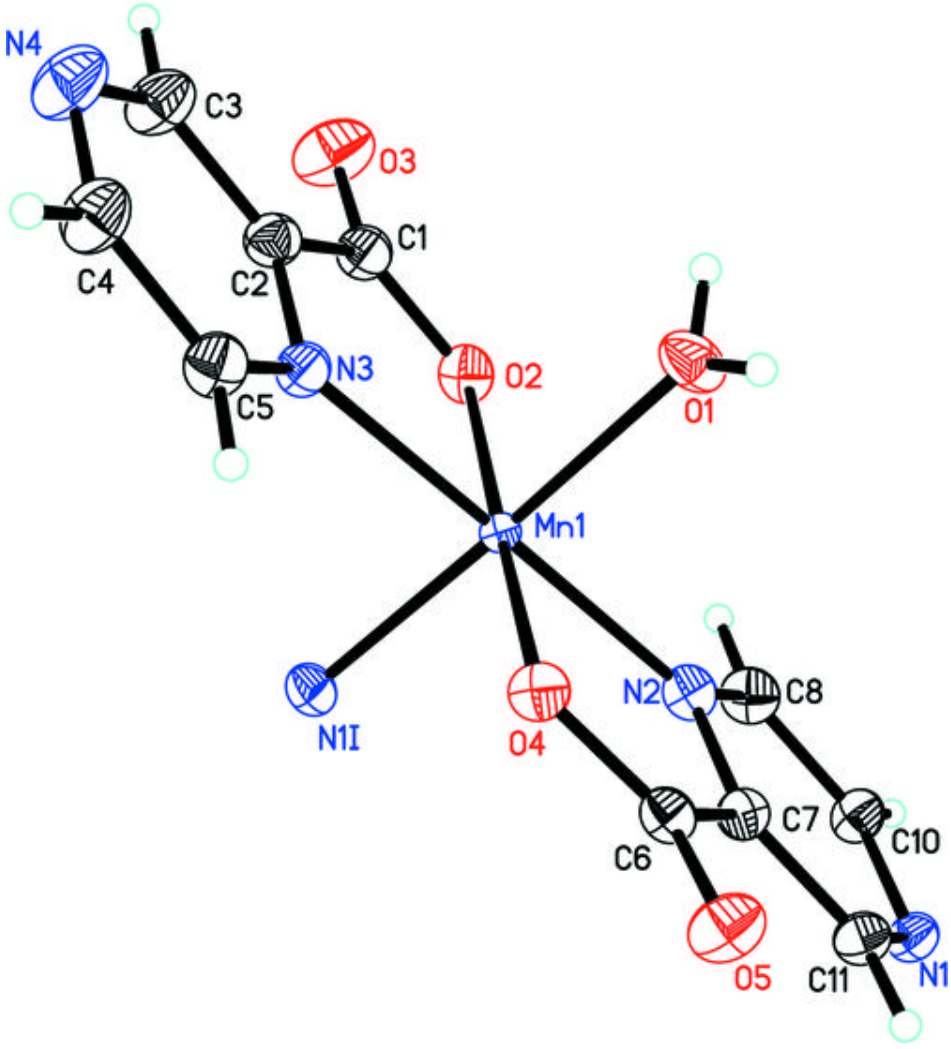

Fig. 2