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catena-Poly[[triaquamanganese(II)]-μ-1,2,4-triazole-3,5-dicarboxylato-$\kappa^3O^3{:}N^4,O^5$]

Yuan-Yuan Liu

Department of Chemistry, Tianjin Normal University, Tainjin 300071, People's Republic of China
Correspondence e-mail: liuyuanyuan1973@yahoo.com.cn

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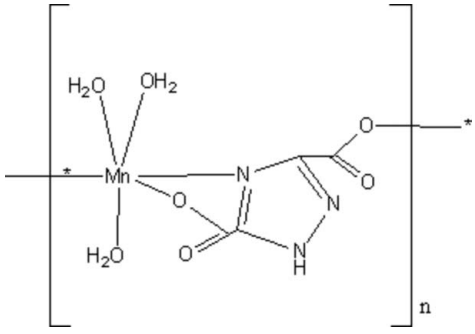
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.021; wR factor = 0.058; data-to-parameter ratio = 11.2.

In the title compound, $[Mn(C_4HN_3O_4)(H_2O)_3]_n$, 1,2,4-triazole-3,5-dicarboxylate ligand adopts a tridentate bridging mode, linking Mn^{II} ions into one-dimensional linear chains. In the crystal structure, intermolecular N—H···O, O—H···N and O—H···O hydrogen bonds involving carboxylate O atoms, triazole groups and water molecules form a three-dimensional network.

Related literature

For background information, see: Batten & Robson (1998); Munakata *et al.*, (1996); Lemoine *et al.*, (2006); Baitalik *et al.* (2004).



Experimental

Crystal data

$[Mn(C_4HN_3O_4)(H_2O)_3]$
M_r = 264.07
Monoclinic, $P2_1/n$
a = 10.8389 (9) Å
b = 6.7367 (6) Å
c = 12.5802 (11) Å
β = 107.546 (1)°
V = 875.85 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.53 mm^{-1}
T = 293 (2) K
0.32 × 0.10 × 0.08 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.861, T_{max} = 0.882
4544 measured reflections
1528 independent reflections
1386 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.058
S = 1.05
1528 reflections
136 parameters
9 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1^{i}	0.86	1.94	2.7674 (18)	162
O5—H5A···O2^{ii}	0.85	1.87	2.6958 (18)	165
O5—H5B···O6^{iii}	0.85	2.23	2.903 (2)	136
O6—H6A···O4	0.85	1.85	2.7019 (19)	175
O6—H6B···O3^{iv}	0.85	1.93	2.7653 (18)	169
O7—H7A···N2^{v}	0.85	2.10	2.921 (2)	163
O7—H7B···O4^{iv}	0.85	2.02	2.8688 (18)	175

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+2, -y+1, -z+1$; (iv) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (v) $-x+1, -y, -z+1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2379).

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supplementary materials

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Y.-Y. Liu

Comment

In the past few decades metal organic coordination compounds have received great interest not only because of their wide application in materials science but also their interesting structural motifs (Batten & Robson, 1998; Munakata *et al.*, 1996). In the rational design and synthesis of these coordiantion polymers, serveral important tuning factors should be considered, such as the ligand functional groups, the metal(II) centers preference and weak but highly directed secondary hydrogen bond interactions. Ligands simultaneously containing O– and N– donor groups are favored *e.g.* pyridine-polycarboxylic acid ligands, imidazole-polycarboxylic acid ligands. These types of ligands have exhibited numerous different coordination modes and form novel coordination polymers with novel properties (Lemoine *et al.*, 2006). Compared to those ligands above, complexes of 1,2,4-triazole-3,5-dicarboxylic acid ligands have been less investigated but a study of these types of complexes has been carried out by Baitalik *et al.* (2004). Mn(II) compounds are also interesting because many Mn(II) compounds exhbit mangnetic properties such as single molecule magnets (SMMS). In this paper, a new one-dimensional complex $[Mn(L)(H_3O)]_n$ (1), where *L* = 3,5-dicarboxylic acid-1,2,4-triazole has been isolated and its single-crystal structure has been determined.

Part of the structure of (I) is shown in Fig. 1. The Mn^{II} ion is in a slightly distorted octahedral coordination geometry formed by three coordinated water molecules, one N atom, one carboxylate O atom in a bidentate mode from one *L* ligand and one carboxylate O atom from a symmetry related *L* Ligand in a monodentate mode. Hence, the *L* ligands adopts a tridentate bridging mode to Mn^{II} ions forming a one-dimensional linear chain structure (Fig. 2). Due to the functional groups of *L*, numerous hydrogen bond interactions are present. In the crystal structure intermolecular N—H···O and O—H···O hydrogen bonds involving carboxylate O atoms, triazole groups and coordinated water molecules form a three-dimensional network.

Experimental

A methanol solution (15 ml) of *L* (0.7 mmol) was slowly added to an aqueous solution (10 ml) of $MnCl_26H_2O$ (0.7 mmol). The resulting solution was stirred and refluxed for 3 h at room temperature. The resulting solution was filtered. After 14 days white prism crystals suitable for *x*-ray diffraction were obtained from the filtrate. elemental analysis, calculated for $C_4H_7MnN_3O_7$: C 18.19, H 2.67, N 15.91%; found: C 18.30, H 2.69, N 15.84%.

Refinement

H atoms were placed in calculated positions with O—H = 0.85 and N—H = 0.86 Å. They were included in the riding-motion approximation with $U_{iso}(H) = 1.2U_{eq}(N)$ and $U_{iso}(H) = 1.5U_{eq}(O)$.

Figures

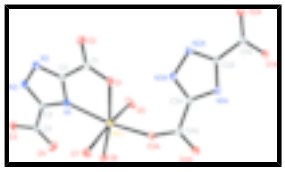

Fig. 1. Part of the one-dimensional chain structure of (I). Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (A) *x* + 1/2, −*y* + 1/2, *z* + 1/2.

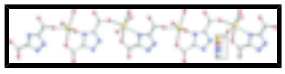

Fig. 2. A section of the one-dimenional chain structure of (I).

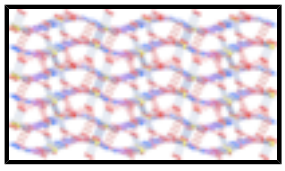

Fig. 3. Part of the crystal structure of (I). Red dashed lines represent O—H···O hydrogen bonds and purple dashed lines represent N—H···O hydrogen bonds.

catena-Poly[[triaquamanganese(II)]-μ-1,2,4-triazole-3,5-dicarboxylato- $\kappa^3O^3:N^4,O^5$]

Crystal data

$[Mn(C_4HN_3O_4)(H_2O)_3]$	F_{000} = 532
M_r = 264.07	D_x = 2.003 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2564 reflections
a = 10.8389 (9) Å	θ = 3.0–27.7º
b = 6.7367 (6) Å	μ = 1.53 mm^{-1}
c = 12.5802 (11) Å	T = 293 (2) K
β = 107.546 (1)º	Prism, colorless
V = 875.85 (13) Å^3	0.32 × 0.10 × 0.08 mm
Z = 4	

Data collection

Bruker APEXII diffractometer	1528 independent reflections
Radiation source: fine-focus sealed tube	1386 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.018
T = 293(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 3.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→12
T_{min} = 0.861, T_{max} = 0.882	k = −7→8
4544 measured reflections	l = −9→14

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.021$	H-atom parameters constrained
$wR(F^2) = 0.058$	$w = 1/[\sigma^2(F_o^2) + (0.0302P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
1528 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
136 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
9 restraints	Extinction correction: SHELXL97
Primary atom site location: constr	Extinction coefficient: 0.257 (15)

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}
Mn1	0.82891 (2)	0.18703 (4)	0.54821 (2)	0.01986 (11)
O1	0.71670 (11)	0.14416 (19)	0.66411 (10)	0.0239 (3)
O2	0.51740 (12)	0.1395 (2)	0.68205 (10)	0.0291 (3)
O3	0.49076 (11)	0.44584 (19)	0.16752 (9)	0.0255 (3)
O4	0.69816 (12)	0.3869 (3)	0.25424 (11)	0.0382 (4)
O5	0.88499 (15)	0.4806 (2)	0.61302 (11)	0.0391 (4)
H5A	0.9132	0.5107	0.6817	0.059*
H5B	0.9115	0.5538	0.5693	0.059*
O6	0.91075 (12)	0.26752 (19)	0.41689 (10)	0.0241 (3)
H6A	0.8465	0.3112	0.3650	0.036*
H6B	0.9509	0.1723	0.3977	0.036*
O7	0.79141 (12)	−0.1105 (2)	0.47093 (10)	0.0274 (3)
H7A	0.7348	−0.1811	0.4875	0.041*
H7B	0.7905	−0.1167	0.4032	0.041*
N1	0.62527 (13)	0.2778 (2)	0.45004 (11)	0.0180 (3)
N2	0.42098 (14)	0.2723 (2)	0.45785 (11)	0.0197 (3)
N3	0.42449 (13)	0.3315 (2)	0.35623 (11)	0.0200 (3)
H3	0.3578	0.3638	0.3019	0.024*
C1	0.59476 (16)	0.1698 (2)	0.63011 (14)	0.0191 (4)
C2	0.54429 (15)	0.2424 (2)	0.51157 (13)	0.0169 (3)
C3	0.54639 (16)	0.3330 (2)	0.35194 (14)	0.0175 (4)
C4	0.58276 (16)	0.3916 (3)	0.25006 (14)	0.0214 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.01684 (16)	0.02659 (18)	0.01511 (16)	−0.00047 (10)	0.00324 (11)	−0.00061 (10)
O1	0.0167 (6)	0.0371 (7)	0.0158 (6)	0.0002 (5)	0.0017 (5)	0.0041 (5)
O2	0.0247 (7)	0.0450 (8)	0.0201 (6)	0.0023 (6)	0.0106 (5)	0.0097 (6)
O3	0.0212 (6)	0.0360 (7)	0.0157 (6)	−0.0045 (5)	0.0000 (5)	0.0057 (5)
O4	0.0223 (7)	0.0673 (10)	0.0258 (7)	0.0048 (7)	0.0086 (6)	0.0159 (7)
O5	0.0610 (10)	0.0352 (8)	0.0237 (7)	−0.0218 (7)	0.0168 (7)	−0.0089 (6)
O6	0.0228 (6)	0.0284 (7)	0.0216 (6)	0.0018 (5)	0.0073 (5)	0.0003 (5)
O7	0.0273 (7)	0.0319 (7)	0.0253 (7)	−0.0069 (6)	0.0117 (5)	−0.0038 (6)
N1	0.0174 (7)	0.0212 (7)	0.0147 (7)	−0.0010 (6)	0.0039 (6)	0.0011 (6)
N2	0.0198 (7)	0.0242 (8)	0.0152 (7)	0.0004 (6)	0.0053 (6)	0.0022 (6)
N3	0.0175 (7)	0.0253 (8)	0.0145 (7)	0.0012 (6)	0.0010 (6)	0.0030 (6)
C1	0.0222 (9)	0.0184 (9)	0.0152 (8)	−0.0011 (7)	0.0035 (7)	−0.0003 (6)
C2	0.0189 (8)	0.0170 (8)	0.0146 (8)	−0.0006 (7)	0.0046 (6)	−0.0014 (7)
C3	0.0172 (8)	0.0188 (8)	0.0155 (8)	−0.0001 (6)	0.0032 (7)	−0.0004 (6)
C4	0.0212 (9)	0.0252 (9)	0.0170 (9)	−0.0018 (7)	0.0047 (7)	0.0013 (7)

Geometric parameters (Å, °)

Mn1—O3^{i}	2.1317 (12)	O6—H6A	0.8501
Mn1—O5	2.1557 (14)	O6—H6B	0.8502
Mn1—O6	2.1665 (12)	O7—H7A	0.8499
Mn1—O1	2.1812 (12)	O7—H7B	0.8499
Mn1—O7	2.2115 (13)	N1—C3	1.325 (2)
Mn1—N1	2.2644 (14)	N1—C2	1.355 (2)
O1—C1	1.272 (2)	N2—C2	1.319 (2)
O2—C1	1.225 (2)	N2—N3	1.3507 (19)
O3—C4	1.258 (2)	N3—C3	1.339 (2)
O3—Mn1^{ii}	2.1317 (12)	N3—H3	0.8600
O4—C4	1.236 (2)	C1—C2	1.507 (2)
O5—H5A	0.8500	C3—C4	1.503 (2)
O5—H5B	0.8501		
O3^{i}—Mn1—O5	92.32 (5)	Mn1—O7—H7A	116.7
O3^{i}—Mn1—O6	101.70 (5)	Mn1—O7—H7B	115.5
O5—Mn1—O6	85.71 (5)	H7A—O7—H7B	115.3
O3^{i}—Mn1—O1	88.86 (5)	C3—N1—C2	103.55 (13)
O5—Mn1—O1	91.09 (5)	C3—N1—Mn1	146.39 (12)
O6—Mn1—O1	169.07 (5)	C2—N1—Mn1	109.49 (10)
O3^{i}—Mn1—O7	86.11 (5)	C2—N2—N3	102.52 (13)
O5—Mn1—O7	172.49 (5)	C3—N3—N2	110.49 (13)
O6—Mn1—O7	87.42 (5)	C3—N3—H3	124.8
O1—Mn1—O7	96.21 (5)	N2—N3—H3	124.8
O3^{i}—Mn1—N1	163.21 (5)	O2—C1—O1	127.34 (16)
O5—Mn1—N1	94.36 (6)	O2—C1—C2	118.63 (15)

O6—Mn1—N1	94.15 (5)	O1—C1—C2	114.02 (15)
O1—Mn1—N1	75.64 (5)	N2—C2—N1	114.30 (14)
O7—Mn1—N1	89.15 (5)	N2—C2—C1	124.48 (15)
C1—O1—Mn1	119.30 (11)	N1—C2—C1	121.21 (14)
C4—O3—Mn1^{ii}	137.63 (12)	N1—C3—N3	109.14 (15)
Mn1—O5—H5A	125.3	N1—C3—C4	127.34 (15)
Mn1—O5—H5B	113.5	N3—C3—C4	123.51 (15)
H5A—O5—H5B	115.5	O4—C4—O3	125.64 (16)
Mn1—O6—H6A	104.1	O4—C4—C3	118.63 (15)
Mn1—O6—H6B	113.0	O3—C4—C3	115.71 (15)
H6A—O6—H6B	114.5		
O3^{i}—Mn1—O1—C1	−168.50 (13)	C3—N1—C2—N2	−0.03 (19)
O5—Mn1—O1—C1	99.19 (13)	Mn1—N1—C2—N2	−173.78 (12)
O6—Mn1—O1—C1	26.4 (3)	C3—N1—C2—C1	178.38 (15)
O7—Mn1—O1—C1	−82.55 (12)	Mn1—N1—C2—C1	4.63 (19)
N1—Mn1—O1—C1	4.98 (12)	O2—C1—C2—N2	−1.5 (3)
O3^{i}—Mn1—N1—C3	−150.53 (19)	O1—C1—C2—N2	177.48 (16)
O5—Mn1—N1—C3	96.3 (2)	O2—C1—C2—N1	−179.79 (16)
O6—Mn1—N1—C3	10.3 (2)	O1—C1—C2—N1	−0.8 (2)
O1—Mn1—N1—C3	−173.7 (2)	C2—N1—C3—N3	0.49 (18)
O7—Mn1—N1—C3	−77.0 (2)	Mn1—N1—C3—N3	169.80 (15)
O3^{i}—Mn1—N1—C2	18.4 (2)	C2—N1—C3—C4	179.80 (16)
O5—Mn1—N1—C2	−94.71 (11)	Mn1—N1—C3—C4	−10.9 (3)
O6—Mn1—N1—C2	179.28 (11)	N2—N3—C3—N1	−0.79 (19)
O1—Mn1—N1—C2	−4.70 (10)	N2—N3—C3—C4	179.86 (15)
O7—Mn1—N1—C2	91.93 (11)	Mn1^{ii}—O3—C4—O4	111.0 (2)
C2—N2—N3—C3	0.72 (18)	Mn1^{ii}—O3—C4—C3	−70.5 (2)
Mn1—O1—C1—O2	174.89 (14)	N1—C3—C4—O4	1.2 (3)
Mn1—O1—C1—C2	−4.03 (19)	N3—C3—C4—O4	−179.56 (17)
N3—N2—C2—N1	−0.42 (19)	N1—C3—C4—O3	−177.38 (16)
N3—N2—C2—C1	−178.77 (15)	N3—C3—C4—O3	1.8 (2)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O1^{ii}	0.86	1.94	2.7674 (18)	162
O5—H5A···O2^{iii}	0.85	1.87	2.6958 (18)	165
O5—H5B···O6^{iv}	0.85	2.23	2.903 (2)	136
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O7—H7B···O4^{v}	0.85	2.02	2.8688 (18)	175

Symmetry codes: (ii) *x*−1/2, −*y*+1/2, *z*−1/2; (iii) −*x*+3/2, *y*+1/2, −*z*+3/2; (iv) −*x*+2, −*y*+1, −*z*+1; (v) −*x*+3/2, *y*−1/2, −*z*+1/2; (vi) −*x*+1, −*y*, −*z*+1.

Fig. 1

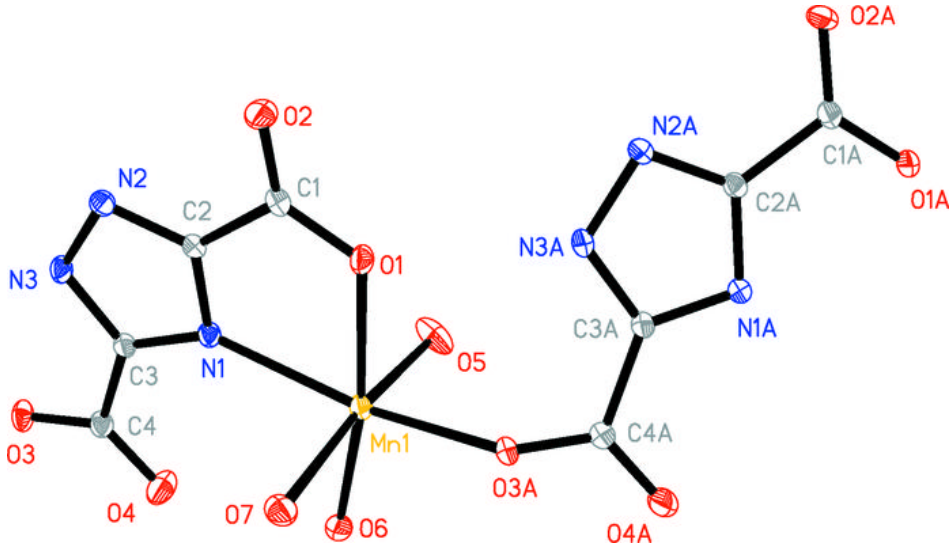
O2A
N2A
C1A
O1A
C2A
N3A
C3A
N1A
O2
C1
N2
C2
N3
O1
C3
N1
O5
C4
O3
Mn1
C4A
O3A
O4
O7
O6
O4A

Fig. 2

Fig. 3