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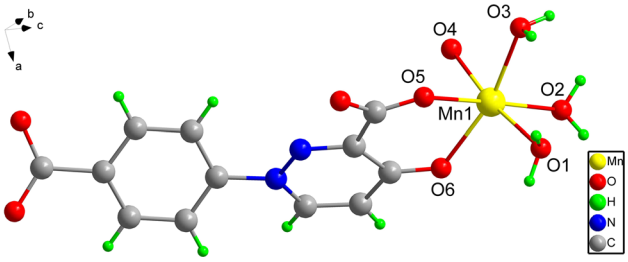
Crystal structure of *catena*-poly[triaqua-(μ$_2$ -1-(4-carboxylatophenyl)-4-oxo-1,4-dihydropyridazine-3-carboxylato-κ^3*O,O′:O″*)manganese(II)], $C_{12}H_{12}N_2O_8Mn$



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Abstract

$C_{12}H_{12}N_2O_8Mn$, orthorhombic, *Pbca* (no. 61), a = 11.5651(15) Å, b = 9.4169(12) Å, c = 25.634(3) Å, V = 2791.7(6) Å^3, Z = 8, $R_{gt}(F)$ = 0.0402, $wR_{ref}(F^2)$ = 0.1166, T = 296.15 K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of material

The mixture of manganese chloride tetrahydrate 19.7 mg (0.1 mmol), 1-(4-carboxyphenyl)-4-oxo-1,4-dihydropyridazine-3-carboxylic acid 26.1 mg (0.1 mmol), NaOH 4 mg (0.1 mmol) and methyl alcohol (10 mL) were placed in a 25 mL vial and heated at 90 °C for 72 h, then cooled to room temperature over 24 h. Light green needle shaped crystals were collected after cooling to room temperature.

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.13 × 0.12 × 0.11 mm
Wavelength:	Cu *K*α radiation (1.5478 Å)
μ:	8.24 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	89.4°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	15593, 3141, 0.051
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 2366
$N(param)_{refined}$:	211
Programs:	Bruker [1], Olex2 [2], SHELX [3, 4]

2 Experimental details

Using Olex2 [2], the structure was solved with the ShelXT [3] structure solution program and refined with the ShelXL [4] refinement package.

3 Comment

Currently, metal coordination polymers composed of various organic ligands and metal ions or metal clusters can be applied in many fields due to their diverse structures and interesting properties [5, 6], for instance, optics [7], gas adsorption/separation [8], catalysis [9], sensing [10], drug transportation [11], etc. However, the diversity in the framework architectures of such coordination polymers counts on many factors, such as the metal atom species, the coordination geometry of metal centers, the coordination ability of organic ligands and the reaction conditions (pH, temperature, solvent and so on) [12, 13], So that the selection of organic ligands and metal ions is the key to constructing fluorescent coordination polymers. For

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.2923 (2)	0.6712 (3)	0.59005 (10)	0.0228 (6)
C2	0.3717 (2)	0.7060 (3)	0.54458 (10)	0.0219 (6)
C3	0.4628 (2)	0.8131 (3)	0.54659 (10)	0.0236 (6)
C4	0.5294 (3)	0.8203 (3)	0.49973 (11)	0.0312 (7)
H4	0.591827	0.882401	0.497844	0.037*
C5	0.5032 (3)	0.7387 (3)	0.45826 (12)	0.0325 (7)
H5	0.546571	0.746765	0.427862	0.039*
C6	0.3779 (3)	0.5580 (3)	0.41657 (11)	0.0309 (7)
C7	0.2636 (3)	0.5223 (5)	0.41248 (16)	0.0648 (14)
H7	0.211121	0.553947	0.437399	0.078*
C8	0.4559 (3)	0.5135 (3)	0.37968 (12)	0.0294 (7)
H8	0.533329	0.539563	0.381956	0.035*
C9	0.4171 (3)	0.4287 (3)	0.33883 (12)	0.0307 (7)
H9	0.469405	0.397983	0.313693	0.037*
C10	0.2261 (3)	0.4397 (5)	0.37155 (15)	0.0595 (13)
H10	0.148067	0.417465	0.368598	0.071*
C11	0.3031 (3)	0.3895 (3)	0.33491(11)	0.0291 (7)
C12	0.2598 (3)	0.2960 (3)	0.29101 (11)	0.0280 (6)
Mn1	0.36334 (4)	0.95586 (5)	0.64587 (2)	0.01942 (14)
N1	0.3500 (2)	0.6281 (3)	0.50324 (9)	0.0286 (6)
N2	0.4142 (2)	0.6446 (3)	0.46022 (9)	0.0308 (6)
O1	0.45305 (19)	0.8768 (2)	0.71313 (8)	0.0375 (5)
H1A	0.410354	0.817143	0.728978	0.056*
H1B	0.511343	0.828568	0.703278	0.056*
O2	0.44593 (19)	1.1634 (2)	0.66523 (8)	0.0327 (5)
H2A	0.500448	1.149972	0.687075	0.049*
H2B	0.397650	1.215423	0.681542	0.049*
O3	0.21166 (19)	0.9802 (2)	0.69732 (8)	0.0354 (5)
H3A	0.218252	0.924746	0.723580	0.053*
H3B	0.211741	1.063485	0.710620	0.053*
O4	0.23373 (19)	0.5605 (2)	0.58568 (8)	0.0331 (5)
O5	0.2890 (2)	0.7528 (2)	0.62855 (9)	0.0391 (6)
O6	0.48274 (17)	0.8921 (2)	0.58492 (8)	0.0294 (5)
O7	0.33282 (19)	0.2251 (3)	0.26576 (9)	0.0420 (6)
O8	0.15416 (18)	0.2982 (3)	0.28066 (9)	0.0441 (6)

example, the incorporation of functional groups including pyridyl, imidazole and carboxyl group into the internal of coordination polymers could enhance the fluorescence sensing capability through various host-guest interactions, for synthesis of coordination polymers with appropriate luminous performance and are vital. Up to now, several complexes constructed by 1-(4-carboxylatophenyl)-4-oxo-1,4-dihydropyridazine-3-carboxylate have been reported, which exhibited structural diversity and different properties [14–17].

The asymmetric unit of the title complex contains one independent Mn(II) ion, one deprotonated 1-(4-carboxyphenyl)-4-oxo-1,4-dihydropyridazine-3-carboxylic acid and three monodentate coordinated water molecules. As show in Figure, each Mn(II) ion is six-coordinated with three oxygen atoms from three monodentate coordinated water molecules and three oxygen atoms from two deprotonated ligands. There exists a dihedral angle of 29.8° between the benzene and pyridazine rings. Among them, the carboxyl group adjacent to pyridazine ring adopts the bridging mode to coordinate the two neighboring Mn(II) ions to form a one-dimensional MnO_6 chain. Meanwhile, the carboxyl oxygen of the benzene ring is not involved in coordination. After further modification of the ligand, an interesting 1D structure was formed, which is linked by intermolecular hydrogen bonding to form a 3D supermolecular structure.

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