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(μ-Formato-κ^2O:O')aquachloro(1,10-phenanthroline-κ^2N,N')manganese(II) monohydrate

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Key indicators

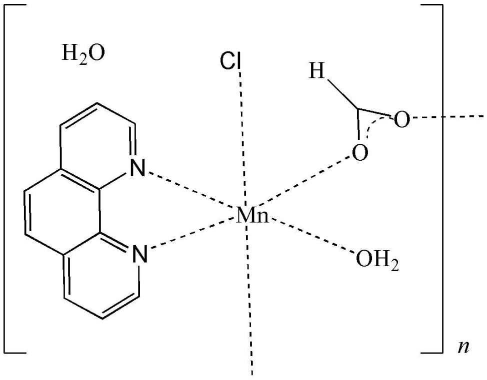
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.046
wR factor = 0.091
Data-to-parameter ratio = 12.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $[MnCl(CHO_2)(C_{12}N_2H_8)(H_2O)]\cdot H_2O$, each Mn^{II} ion is coordinated by two O atoms from two formate anions, a water molecule, a Cl$^-$ anion and two N atoms of the 1,10-phenanthroline ligand, forming an octahedral environment. The formate anions function as bridges between the Mn^{II} ions, resulting in a zigzag chain structure along the [001] direction.

Comment

The structural design or modification of coordination polymer frameworks has become a very active field, owing to the crystallographic diversity of these compounds and their promising applications in catalysis, gas adsorption and nonlinear optics (Eddaoudi *et al.*, 2001; Swiegers & Malefetse, 2000). In this field, popular bridging ligands are polycarboxylic acids and their derivatives. Numerous coordination polymers with one-, two- and three-dimensional framework structures have been prepared (Luo *et al.*, 2003; Rosi *et al.*, 2003). However, only a few coordination polymers assembled by the monocarboxylate bridge of the formate anion have been documented to date (Halvorson *et al.*, 1990; van Albada *et al.*, 1999). In an extension of this research, we report here the crystal structure of the title compound, (I).



(I)

In compound (I), the Mn^{II} ion has a six-coordinate environment, defined by two O atoms from two formate anions, a water molecule, a Cl$^-$ anion and two N atoms of the 1,10-phenanthroline ligand in an octahedral geometry (Fig. 1 and Table 1). The equatorial plane is formed by four atoms, O1, O3, N1 and N2, with near-planarity (r.m.s. deviation 0.0406 Å). The two axial sites are occupied by atoms Cl1 and O2.

All the formate anions of (I) are in the μ_2-bridging coordination mode, while in the previously reported complex

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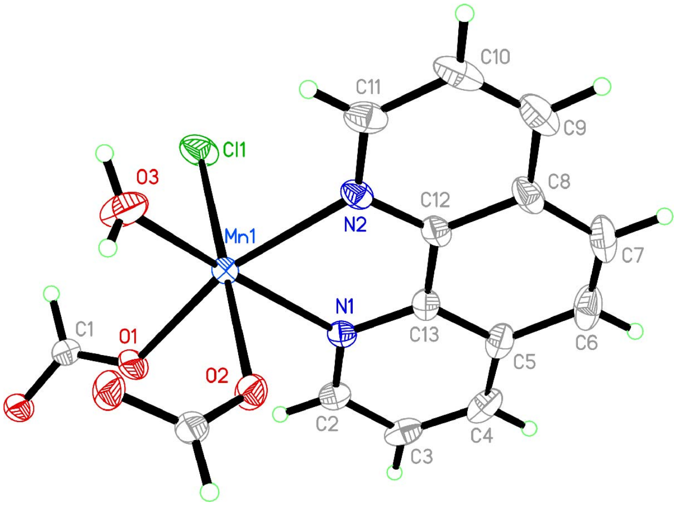

Figure 1
The coordination environment of the Mn^{II} ion in (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. The uncoordinated water molecule has been omitted for clarity.

$[Cu(C_5H_6N_2)_2(CHO_2)_2]$ there is one monodentate formate anion and one μ_2-bridging formate anion (van Albada *et al.*, 1999). Moreover, each $[MnCl(C_{12}N_2H_8)(H_2O)]^+$ cation is linked to its two neighbours by two formate anions, resulting in a zigzag chain structure with an Mn···Mn^i separation of 5.5364 (10) Å along the [001] direction [symmetry code: (i) $1 - x$, $1 - y$, $z + \frac{1}{2}$; Fig. 2].

In the crystal structure of (I), O—H···Cl and O—H···O hydrogen-bond interactions support the above-mentioned zigzag chain (Table 2).

Experimental

The title compound was synthesized by the hydrothermal method from a mixture of 1,10-phenanthroline (2 mmol, 0.36 g), $MnCl_2·2H_2O$ (1 mmol, 0.16 g), formic acid (1 mmol, 0.05 g) and water (20 ml) in a 30 ml Teflon-lined stainless steel reactor. The resulting solution was heated to 412 K for 5 d. After the reaction, the system was slowly cooled to room temperature; pink block-shaped crystals of (I) were collected and washed with distilled water.

Crystal data

$[MnCl(CHO_2)(C_{12}N_2H_8)(H_2O)]·H_2O$
$M_r = 351.64$
Orthorhombic, $Pna2_1$
$a = 19.2667$ (17) Å
$b = 11.1275$ (10) Å
$c = 6.6484$ (6) Å
$V = 1425.4$ (2) Å^3
$Z = 4$

$D_x = 1.639$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1721 reflections
$\theta = 2.7$–$24.1°$
$\mu = 1.13$ mm^{-1}
$T = 298$ (2) K
Block, pink
0.28 × 0.16 × 0.10 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.743$, $T_{max} = 0.895$
7289 measured reflections

2546 independent reflections
2362 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 25.3°$
$h = -23 \rightarrow 23$
$k = -13 \rightarrow 8$
$l = -7 \rightarrow 7$

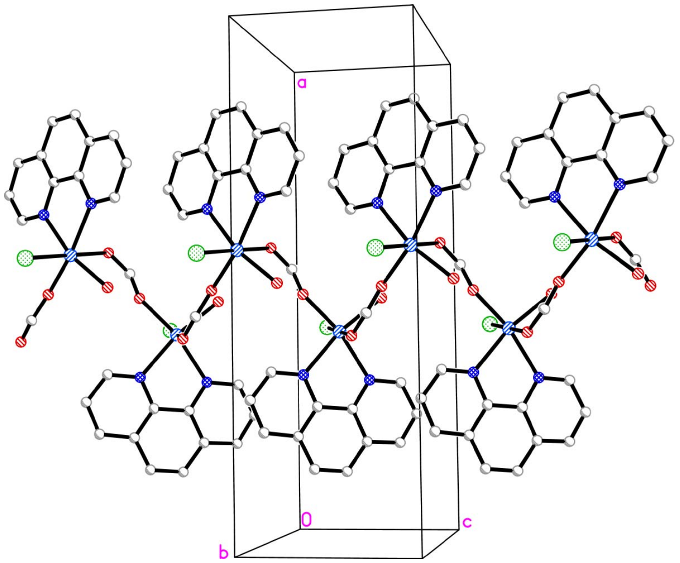

Figure 2
The zigzag chain structure of (I) along the [001] direction. The uncoordinated water molecule and all H atoms have been omitted for clarity.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.091$
$S = 1.10$
2546 reflections
202 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0251P)^2 + 1.2405P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Absolute structure: Flack (1983), with 1142 Friedel pairs
Flack parameter: 0.26 (3)

Table 1
Selected geometric parameters (Å, °).

Mn1—O3	2.132 (3)	Mn1—N2	2.272 (3)
Mn1—O2	2.138 (3)	Mn1—Cl1	2.5146 (13)
Mn1—N1	2.250 (4)	Mn1—Mn1^i	5.5364 (10)
Mn1—O1	2.258 (3)		
O3—Mn1—O2	96.38 (15)	N1—Mn1—N2	74.19 (13)
O3—Mn1—N1	166.00 (15)	O1—Mn1—N2	89.31 (12)
O2—Mn1—N1	91.84 (13)	O3—Mn1—Cl1	93.10 (11)
O3—Mn1—O1	86.86 (13)	O2—Mn1—Cl1	96.06 (9)
O2—Mn1—O1	83.71 (12)	N1—Mn1—Cl1	97.28 (9)
N1—Mn1—O1	82.79 (12)	O1—Mn1—Cl1	179.76 (10)
O3—Mn1—N2	96.36 (16)	N2—Mn1—Cl1	90.93 (9)
O2—Mn1—N2	165.10 (13)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3B···O2^i	0.81 (2)	1.98 (2)	2.709 (5)	150 (4)
O3—H3A···O4^i	0.80 (2)	1.91 (2)	2.672 (5)	162 (5)
O4—H4B···Cl1^{ii}	0.82 (2)	2.41 (2)	3.229 (4)	177 (4)
O4—H4A···Cl1^i	0.84 (2)	2.35 (3)	3.128 (4)	155 (4)

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

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The H atoms of the water molecules were located in difference Fourier maps and refined, with O—H and H···H distances restrained to be 0.82 (2) and 1.39 (1) Å, respectively, and with $U_{iso}(H) = 1.2U_{eq}(O)$. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.93 Å, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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, 2002); software used to prepare material for publication: *SHELXL97*.

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