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Tetraaquabis(5-fluorouracil-1-acetato)manganese(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.093
Data-to-parameter ratio = 11.0

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

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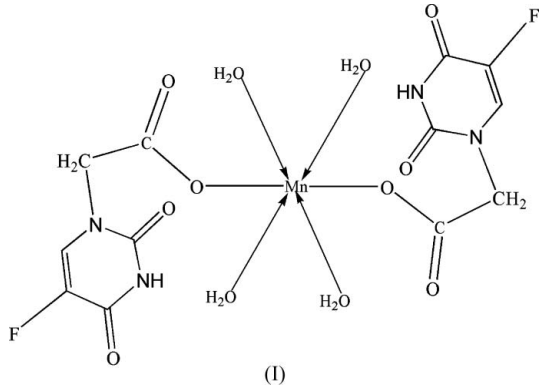
In the centrosymmetric title compound, $[Mn(C_6H_4N_2O_4F)_2(H_2O)_4]$, each Mn^{II} ion is coordinated by two 5-fluorouracil-1-acetate anions *via* the carboxylate O atoms and four water molecules, forming a six-coordinate octahedral environment. N—H···O and O—H···O hydrogen-bonding interactions link adjacent molecules into a three-dimensional network.

Comment

5-Fluorouracil (5-FU) is an antimetabolite with good antimicrobial and antitumor activity, but its administration is accompanied by significant toxic side effects and delivery problems (Ouchi *et al.*, 1997; Nichifor & Schacht, 1994; Nichifor *et al.*, 1997; Hulme *et al.*, 2005). In order to improve the topical delivery of 5-FU and reduce the side effects, many derivatives of 5-FU have been synthesized, some of which have better biological activity. 5-Fluorouracil-1-acetic acid (5-FUAA) is a member of this family (Sloan *et al.*, 1993; Li *et al.*, 2000; Beall & Sloan, 2001; Beall & Sloan, 2002). As increasing attention has been paid to the anticancer activity of 5-FU and its derivatives (Akgerman & Guney, 2000), several transition metal complexes have been reported (Wang *et al.*, 1993; Huang *et al.*, 2000; Hu *et al.*, 2005). The manganese derivative adduct, $Mn(C_6H_4N_2O_4F)_2(H_2O)_4$, (I), is reported here to build on these studies.



(I)

Mononuclear (I) consists of an Mn atom, four coordinated water molecules and two 5-fluorouracil-1-acetate anions, which bind through their carboxylate O atoms. The Mn atom lies on an inversion center and the geometry around the Mn ion is octahedral (Fig. 1 and Table 1). A square plane is formed by atoms O5, $O5^i$, O6 and $O6^i$ [symmetry code: (i) $-x$, $-y$, $-z+1$], which is crystallographically required to be planar. The N—H···O and O—H···O hydrogen bonds link the mononuclear units to form a three-dimensional network (Fig. 2 and Table 2).

Experimental

5-Fluorouracil-1-acetic acid (2 mmol, 0.75 g) and 1,3-di(4-pyridyl)-propane (2 mmol, 0.40 g) were dissolved in a mixture of water (2 ml) and ethanol (8 ml). The solution was then added dropwise to a stirred aqueous solution (10 ml) of $MnCl_2{\cdot}2H_2O$ (1 mmol, 0.16 g). The resulting solution was filtered and allowed to evaporate slowly at room temperature. After four weeks, prismatic pink crystals of (I) appeared.

Crystal data

$[Mn(C_6H_4N_2O_4F)_2(H_2O)_4]$
M_r = 501.23
Monoclinic, $P2_1/c$
a = 13.1820 (13) Å
b = 5.1106 (5) Å
c = 14.2202 (14) Å
β = 99.809 (2)°
V = 943.98 (16) Å^3
Z = 2
D_x = 1.763 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2209 reflections
θ = 2.9–25.2°
μ = 0.79 mm^{-1}
T = 298 (2) K
Prism, pink
0.32 × 0.16 × 0.13 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.786, T_{max} = 0.904
4685 measured reflections
1687 independent reflections
1619 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 25.2°
$h = -15 \rightarrow 15$
$k = -6 \rightarrow 5$
$l = -17 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.093
S = 1.16
1687 reflections
154 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0419P)^2 + 0.5989P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O5	2.1563 (18)	Mn1—O6	2.2148 (18)
Mn1—O1	2.1620 (16)		
O5—Mn1—O1^{i}	89.83 (7)	O5^{i}—Mn1—O6	92.57 (7)
O5—Mn1—O1	90.17 (7)	O1^{i}—Mn1—O6	85.81 (7)
O5—Mn1—O6	87.43 (7)	O1—Mn1—O6	94.19 (7)

Symmetry codes: (i) $-x, -y, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O4^{ii}	0.86	1.99	2.843 (3)	175
O6—H6A···O3^{iii}	0.83 (2)	2.02 (2)	2.834 (3)	170 (2)
O6—H6B···O2^{i}	0.81 (2)	1.91 (2)	2.699 (3)	163 (2)
O5—H5A···O1^{iv}	0.84 (2)	1.82 (2)	2.656 (2)	174 (2)
O5—H5B···O3^{v}	0.82 (2)	1.98 (2)	2.788 (2)	170 (2)

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

Water H atoms were located in difference density maps and refined with O—H and H···H distances restrained to 0.82 (2) Å and 1.39 (1) Å, respectively, with U_{iso}(H) = 1.2U_{eq}(parent atom). The other H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of Csp^2—H = 0.93 Å with U_{iso}(H) = 1.2U_{eq}(C), Csp^3—H = 0.97 Å with U_{iso}(H) = 1.5U_{eq}(C), and N—H = 0.86 Å with U_{iso}(H) = 1.2U_{eq}(N).

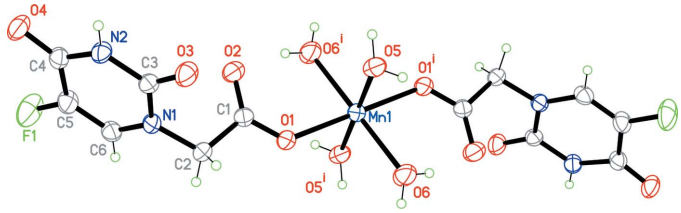


Figure 1
The molecular structure of (I), showing the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $-x, -y, -z+1$.]

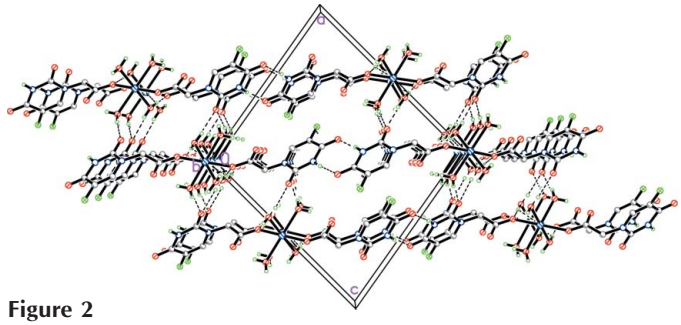


Figure 2
The three-dimensional network formed by hydrogen-bonding interactions, which are shown as dashed lines.

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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