Crystal structure of tetraaquamanganese succinate, $Mn(H_2O)_4C_4H_4O_4$

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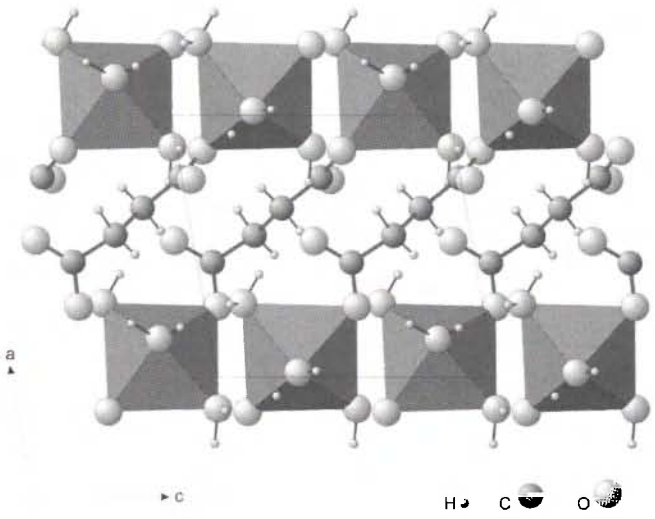

Abstract

$C_4H_{12}MnO_8$, monoclinic, $P12_1/c1$ (No. 14), $a = 7.513(2)$ Å, $b = 14.915(3)$ Å, $c = 7.891(2)$ Å, $\beta = 99.94(2)°$, $V = 871.0$ Å^3, $Z = 4$, $R_{gt}(F) = 0.037$, $wR_{ref}(F^2) = 0.089$, $T = 293$ K.

Source of material

Crystals of $Mn(H_2O)_4(C_4H_4O_4)$ were obtained by controlled evaporation from an aqueous solution of the reaction product of succinic acid and manganese carbonate in water at room temperature.

Discussion

The title compound is the monoclinic modification of triclinic $Mn(H_2O)_4(C_4H_4O_4)$ as described by Gupta et al. [1]. It is isotypic with $Co(H_2O)_4(C_4H_4O_4)$ [2] and $Ni(H_2O)_4(C_4H_4O_4)$ [3]. The structure consists of chains of succinate molecules along [101] which are connected by manganese octahedra. The chains are linked to each other by hydrogen bonds. The conformation of the succinate molecules is *trans*, the torsion angle C1–C2–C3–C4 being 175.11°. The structure is displayed along [001] for $0 < y < 1/2$.

Table 1. Data collection and handling.

Crystal:	pink prism, size 0.06 × 0.12 × 0.18 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	15.31 cm^{-1}
Diffractometer, scan mode:	Enraf Nonius Kappa CCD, 113 frames with $\Delta\varphi = 2$, 30 s per frame (detector distance 28 mm) φ-scan and ω-scan
$2\theta_{max}$:	64.06°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8267, 2912
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2290
$N(param)_{refined}$:	167
Programs:	SHELXS-97 [4], SHELXL-97 [5], ATOMS [6]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(21)	4e	–0.284(3)	0.315(2)	–0.222(3)	0.040(6)
H(22)	4e	–0.442(3)	0.306(2)	–0.124(3)	0.041(6)
H(31)	4e	–0.370(3)	0.461(2)	–0.306(3)	0.035(6)
H(32)	4e	–0.540(3)	0.449(2)	–0.214(3)	0.041(6)
HW(11)	4e	0.029(4)	0.540(2)	0.358(4)	0.065(9)
HW(12)	4e	–0.075(5)	0.503(3)	0.209(5)	0.10(1)
HW(21)	4e	0.187(4)	0.188(2)	0.243(4)	0.052(8)
HW(22)	4e	0.193(4)	0.194(2)	0.408(4)	0.058(9)
HW(31)	4e	–0.124(4)	0.290(2)	0.519(4)	0.057(9)
HW(32)	4e	–0.217(4)	0.352(2)	0.450(4)	0.044(8)
HW(41)	4e	0.363(5)	0.368(2)	0.208(4)	0.07(1)
HW(42)	4e	0.283(4)	0.426(2)	0.095(4)	0.057(8)

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mn(1)	4e	0.07330(3)	0.35587(2)	0.31062(3)	0.0181(2)	0.0242(2)	0.0153(1)	0.00056(9)	–0.0018(1)	–0.00134(9)
O(11)	4e	–0.1337(2)	0.33249(9)	0.0895(2)	0.0275(6)	0.0295(7)	0.0207(6)	0.0032(5)	–0.0089(5)	–0.0023(5)
O(12)	4e	–0.2453(2)	0.46868(9)	0.0308(2)	0.0419(8)	0.0271(7)	0.0259(6)	0.0031(6)	–0.0107(6)	–0.0022(5)
O(41)	4e	–0.7304(2)	0.37121(9)	–0.4549(2)	0.0180(6)	0.0465(8)	0.0178(6)	–0.0056(5)	–0.0029(5)	–0.0022(5)
O(42)	4e	–0.4790(2)	0.36898(9)	–0.5666(2)	0.0198(6)	0.0449(8)	0.0220(6)	0.0032(5)	0.0001(5)	–0.0019(5)
C(1)	4e	–0.2368(2)	0.3876(1)	–0.0038(2)	0.0194(8)	0.0271(9)	0.0164(7)	–0.0007(7)	–0.0012(6)	0.0003(6)
C(2)	4e	–0.3549(3)	0.3494(1)	–0.1624(2)	0.0273(9)	0.0271(9)	0.0192(8)	0.0009(7)	–0.0066(7)	–0.0005(7)
C(3)	4e	–0.4582(3)	0.4204(1)	–0.2773(2)	0.0241(8)	0.0271(9)	0.0217(8)	0.0004(7)	–0.0067(7)	–0.0018(7)
C(4)	4e	–0.5614(2)	0.3838(1)	–0.4444(2)	0.0189(8)	0.0198(8)	0.0191(7)	0.0008(6)	–0.0040(6)	0.0021(6)

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Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
OW(1)	4*e*	0.0178(2)	0.4990(1)	0.2954(2)	0.0388(8)	0.0258(7)	0.0329(8)	0.0038(6)	–0.0071(7)	–0.0069(6)
OW(2)	4*e*	0.1439(2)	0.21325(9)	0.3187(2)	0.0424(8)	0.0285(7)	0.0195(6)	0.0094(6)	0.0014(6)	0.0012(5)
OW(3)	4*e*	–0.1203(2)	0.3405(1)	0.4849(2)	0.0172(6)	0.0318(8)	0.0265(7)	–0.0002(5)	0.0010(5)	0.0041(5)
OW(4)	4*e*	0.2798(2)	0.3729(1)	0.1376(2)	0.0274(7)	0.0275(7)	0.0209(6)	–0.0018(5)	0.0001(6)	–0.0002(5)

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