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Key indicators

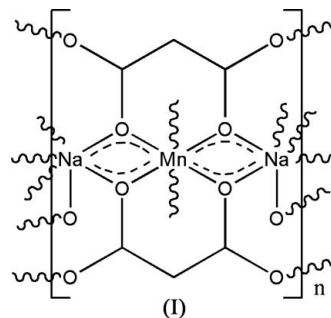
Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.022
 wR factor = 0.064
Data-to-parameter ratio = 10.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Poly[di-aqua-di- μ -malonato-manganese(II)-
disodium(I)]

The title compound, $[\text{Na}_2\text{Mn}(\text{C}_3\text{H}_2\text{O}_4)_2(\text{H}_2\text{O})_2]_n$, obtained by the hydrothermal reaction of $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$, NaOH and malonic acid, is a three-dimensional polymeric complex bridged by malonate dianions. The Mn^{II} atom, which occupies an inversion centre, has distorted octahedral coordination, with $\text{Mn}-\text{O}$ bonds in the range 2.1168 (10)–2.2666 (10) \AA . The Na^{I} atom has slightly distorted octahedral coordination, with $\text{Na}-\text{O}$ distances ranging from 2.3700 (14) to 2.6117 (12) \AA .

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Comment

Metal-organic frameworks (MOFs) have been successfully constructed and self-assembled by metal ions and well designed organic ligands. They have attracted considerable attention in the fields of supramolecular chemistry and crystal engineering due to their unique properties and potential applications (Batten & Murray, 2003; Erxleben, 2003; Kesani & Lin, 2003). In an attempt to investigate the design and control of the self-assemblies of MOFs, we have successfully developed and constructed intriguing MOFs based on rigid or flexible ligands (Wang *et al.*, 2005*a,b*; Wang *et al.*, 2005). Malonic acid was adopted to construct MOFs, which probably results in the versatile structure of coordination polymers, although malonic acid has been widely used in the construction of supramolecules or MOFs (Guo & Guo, 2006; Liu & Xu, 2004; Shen, 2003; Zhang & Lu, 2004; Zhao & Wu, 2005). In this work, we report the structure of $[\text{Na}_2\text{Mn}(\text{C}_3\text{H}_2\text{O}_4)_2(\text{H}_2\text{O})_2]_n$, (I), obtained by the hydrothermal reaction of $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$, NaOH and malonic acid; it is a three-dimensional polymeric complex bridged by malonate dianions.



It is noteworthy that the malonate ligand exhibits versatile coordination modes and links two Mn^{II} and four Na^{I} atoms. The Mn^{II} atom occupies an inversion centre and is chelated by two malonate ligands; two other malonates are involved in monodentate coordination of the Mn^{II} atom, thus completing its octahedral coordination environment with $\text{Mn}-\text{O}$ bonds in

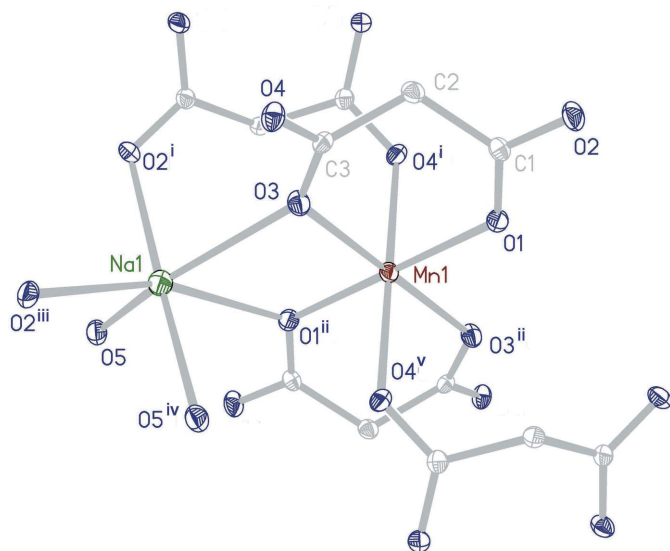


Figure 1
Part of the polymeric structure of (I), showing the atom-numbering scheme (symmetry codes as in Table 1). H atoms are omitted for clarity.

the range 2.1168 (10)–2.2666 (10) Å (Table 1). The Na^I atom also has distorted octahedral coordination, with Na–O distances ranging from 2.3700 (14) to 2.6117 (12) Å, formed by four carboxylate O atoms of four malonate ligands and two water molecules (Fig. 1). Thus, a three-dimensional structure has been constructed by malonate ligands (Fig. 2). A similar coordination mode was reported for [Na₂Zn(C₃H₂O₄)₂·(H₂O)₂]_n (Lin *et al.*, 2003).

Experimental

Malonic acid (0.104 g, 1 mmol) in an aqueous solution (6 ml) of NaOH (0.080 g, 2 mmol) was mixed with an aqueous solution (6 ml) of MnCl₂·4H₂O (0.199 g, 1 mmol). The mixture was placed in a 23 ml Teflon-lined autoclave and heated at 413 K for 120 h. The autoclave was cooled over a period of 12 h at a rate of 5 K h⁻¹. Pale-yellow crystals were collected by filtration, washed with water, and dried in air (yield 221 mg, 65%). Analysis calculated: C 21.13, H 2.36%; found: C 21.07, H 3.40%. IR data (cm⁻¹): 3391 (*m*), 1585 (*s*), 1533 (*s*), 1465 (*m*), 1248 (*m*).

Crystal data

[Na ₂ Mn(C ₃ H ₂ O ₄) ₂ (H ₂ O) ₂]	Mo Kα radiation
<i>M_r</i> = 341.04	Cell parameters from 100 reflections
Orthorhombic, <i>Pbca</i>	$\theta = 3\text{--}15^\circ$
<i>a</i> = 6.8235 (5) Å	$\mu = 1.36\text{ mm}^{-1}$
<i>b</i> = 9.5334 (6) Å	<i>T</i> = 293 (2) K
<i>c</i> = 16.4932 (11) Å	Block, pale yellow
<i>V</i> = 1072.90 (13) Å ³	0.43 × 0.33 × 0.33 mm
<i>Z</i> = 4	
<i>D_x</i> = 2.111 Mg m ⁻³	

Data collection

Bruker SMART CCD area-detector diffractometer	1054 independent reflections
φ and ω scans	994 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	<i>R_{int}</i> = 0.016
<i>T_{min}</i> = 0.569, <i>T_{max}</i> = 0.636	θ_{max} = 26.0°
5267 measured reflections	<i>h</i> = -8 → 8
	<i>k</i> = -11 → 9
	<i>l</i> = -15 → 20

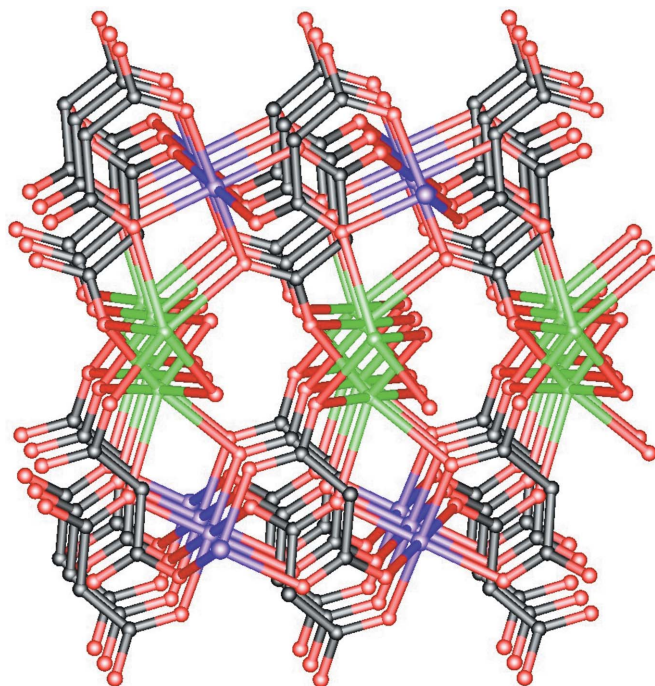


Figure 2
The molecular packing of (I) viewed approximately along the *a* axis (Dolomanov *et al.*, 2003). H atoms have been omitted for clarity. Colour key: black, red, green and blue indicate C, O, Na and Mn atoms, respectively.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0392P)^2 + 0.4117P]$
$R[F^2 > 2\sigma(F^2)] = 0.022$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.064$	$(\Delta/\sigma)_{\text{max}} < 0.001$
<i>S</i> = 1.08	$\Delta\rho_{\text{max}} = 0.26\text{ e \AA}^{-3}$
1054 reflections	$\Delta\rho_{\text{min}} = -0.26\text{ e \AA}^{-3}$
104 parameters	
All H-atom parameters refined	

Table 1

Selected geometric parameters (Å, °).

Mn1–O1	2.1168 (10)	Na1–O2 ⁱⁱⁱ	2.4944 (13)
Mn1–O3	2.1678 (10)	Na1–O3	2.6118 (12)
Mn1–O4 ⁱ	2.2666 (10)	Na1–O5	2.4018 (14)
Na1–O1 ⁱⁱ	2.5713 (12)	Na1–O5 ^{iv}	2.3700 (14)
Na1–O2 ⁱ	2.4148 (13)		
O1–Mn1–O3 ⁱⁱ	91.07 (4)	O2 ⁱ –Na1–O2 ⁱⁱⁱ	101.47 (4)
O1–Mn1–O3	88.93 (4)	O5 ^{iv} –Na1–O1 ⁱⁱ	83.39 (4)
O1–Mn1–O4 ⁱ	85.74 (4)	O5–Na1–O1 ⁱⁱ	79.67 (4)
O1 ⁱⁱ –Mn1–O4 ⁱ	94.26 (4)	O2 ⁱ –Na1–O1 ⁱⁱ	96.83 (4)
O3–Mn1–O4 ⁱ	87.75 (4)	O2 ⁱⁱⁱ –Na1–O1 ⁱⁱ	161.46 (4)
O3–Mn1–O4 ^v	92.25 (4)	O5 ^{iv} –Na1–O3	90.11 (5)
O5 ^{iv} –Na1–O5	103.09 (5)	O5–Na1–O3	147.40 (5)
O5 ^{iv} –Na1–O2 ⁱ	177.47 (5)	O2 ⁱ –Na1–O3	87.57 (4)
O5–Na1–O2 ⁱ	79.42 (4)	O2 ⁱⁱⁱ –Na1–O3	111.13 (4)
O5 ^{iv} –Na1–O2 ⁱⁱⁱ	78.44 (4)	O1 ⁱⁱ –Na1–O3	72.31 (4)
O5–Na1–O2 ⁱⁱⁱ	100.76 (5)		

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

H atoms were located in a difference Fourier map and refined isotropically. The C–H distances are 0.899 (19) and 0.936 (18) Å, and the O–H distances 0.80 (3) and 0.83 (3) Å.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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