Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

catena-Poly[[bis(*N*,*N*-dimethylformamide)-manganese(II)]-di-μ_2-oxalato]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.026
wR factor = 0.076
Data-to-parameter ratio = 18.2

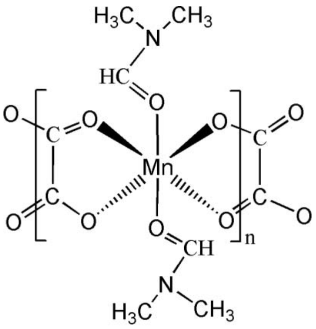
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title complex, $[Mn(C_2O_4)(C_3H_7NO)_2]_n$, forms extended one-dimensional chains with oxalate dianions bridging Mn^{II} atoms in a bis-bidentate mode. The unique Mn^{II} atom lies on a crystallographic twofold axis and is in a distorted octahedral coordination environment. There is a single weak intramolecular C—H···O hydrogen-bond interaction [H···O = 2.38 Å].

Received 23 November 2006
Accepted 28 November 2006

Comment

Supramolecular coordination chemistry has been widely investigated during the last few years due to the interesting architectures, amazing properties and potential technological applications of the materials which can be prepared (Janiak, 2003; Navarro *et al.*, 2006). Recently, Garcia-Couceiro *et al.* (2005) have successfully isolated single-chain one-dimensional coordination polymers $[Mn(ox)(4atr)_2]_n$ and $\{[Co(ox)(Htr)_2]\cdot 2H_2O\}_n$ (ox = oxalate dianion, 4atr = 4-amine-1,2,4-triazole and Htr = 1,2,4-triazole) on different surfaces, affording the possibility to perform nanoscale studies on their properties and investigate their potential applications as nanomaterials. To a further exploration of the coordination chemistry of the oxalate dianion, we report here the crystal structure of the title compound, (I).



(I)

A fully coordinated Mn^{II} atom of (I) is shown in Fig. 1 and selected bond lengths and angles are listed in Table 1. The Mn^{II} atom, lying on a crystallographic twofold rotation axis, is in a distorted octahedral coordination environment involving two carbonyl O atoms from two different dimethylformamide ligands and four carboxylate O atoms from two oxalate dianions. The oxalate dianions act in a bis-bidentate mode, bridging symmetry-related Mn^{II} atoms to form an extended one-dimensional structure (Fig. 2). The intrachain Mn···Mn distance is 5.672 (2) Å. The dimethylformamide ligands coordinate to Mn1 in a monodendate mode. In addtion, there is a single weak C—H···O hydrogen bond (Table 2).

Experimental

To an ethanol solution (5 ml) of oxalic acid (9 mg, 0.1 mmol) was added dropwise a solution (5 ml) of manganese(II) chloride tetrahydrate (19.7 mg, 0.1 mmol) in *N*,*N*-dimethylformamide (10 ml) with stirring. The reaction was stirred at room temperature for about 20 min and then the precipitate was filtered off, leaving the colorless filtrate to evaporate at room temperature. Pink block-shaped crystals suitable for X-ray diffraction were obtained within 6 d in 40% yield. Analysis calculated for $C_4H_7Mn_{0.5}NO_3$: C 33.23, H 4.88, N 9.69%; found: C 33.39, H 4.96, N 9.76%.

Crystal data

$[Mn(C_2O_4)(C_3H_7NO)_2]$
$M_r = 289.16$
Orthorhombic, *Pbcn*
$a = 15.324$ (7) Å
$b = 7.936$ (4) Å
$c = 10.079$ (5) Å
$V = 1225.7$ (10) Å^3
$Z = 4$
$D_x = 1.567$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.10$ mm^{-1}
$T = 293$ (2) K
Block, pink
0.24 × 0.23 × 0.22 mm

Data collection

Bruker APEX-II diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.777$, $T_{\max} = 0.786$
7513 measured reflections
1455 independent reflections
1137 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.027$
$\theta_{\max} = 27.8°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.077$
$S = 1.04$
1455 reflections
80 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2 + 0.3835P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.009$
$\Delta\rho_{\max} = 0.28$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—O2$^{\rm i}$	2.1762 (14)	Mn1—O3	2.1962 (14)
Mn1—O1	2.1828 (15)		
O2$^{\rm i}$—Mn1—O2$^{\rm ii}$	96.02 (8)	O1—Mn1—O3$^{\rm iii}$	99.35 (6)
O2$^{\rm i}$—Mn1—O1$^{\rm iii}$	75.79 (5)	O2$^{\rm i}$—Mn1—O3	92.43 (6)
O2$^{\rm i}$—Mn1—O1	100.14 (6)	O1—Mn1—O3	85.05 (5)
O1$^{\rm iii}$—Mn1—O1	174.05 (7)	O3$^{\rm iii}$—Mn1—O3	85.46 (8)
O2$^{\rm i}$—Mn1—O3$^{\rm iii}$	160.13 (5)		

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

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C4—H4*C*⋯O3	0.96	2.38	2.773 (2)	104

H atoms were located in difference maps, but were subsequently placed in calculated positions and included in the riding-model approximation, with C—H = 0.93–0.96 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or $1.5U_{\rm eq}$(methyl C).

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2001); 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, 2001); software used to prepare material for publication: *SHELXTL* (Bruker, 2001) and *DIAMOND* (Brandenburg & Berndt, 1999).

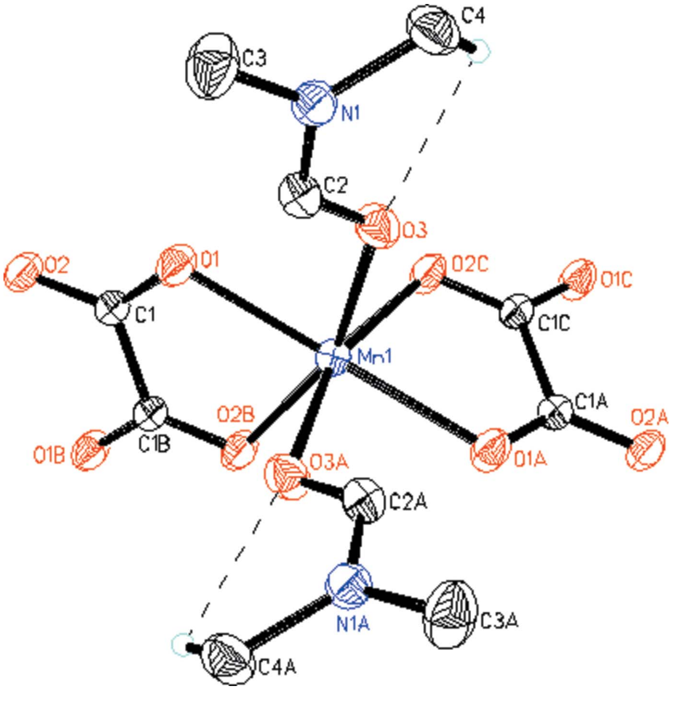


Figure 1
A portion of the one-dimensional structure of the title complex. Displacement ellipsoids are drawn at the 30% probability level. Only H atoms involved in hydrogen bonds are shown. Dashed lines indicate hydrogen bonds. [Symmetry codes: (A) $x, -y, z - \frac{1}{2}$; (B) $-x + 1, -y, -z + 2$; (C) $-x + 1, y, -z + \frac{3}{2}$.]

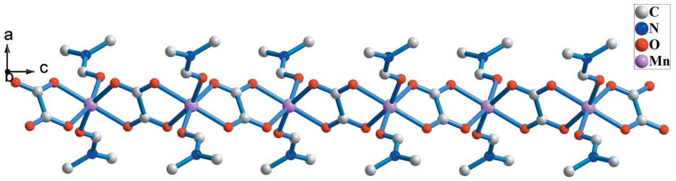


Figure 2
Part of the one-dimensional chain of (I). H atoms have been omitted.

The authors gratefully acknowledge financial support from the National Natural Science Foundation of China (No. 20571056), the Youth fund of Tianjin Normal University (XGW) and the Natural Science Foundation of Tianjin (No. 06YFJMJC03900).

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