Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[μ_3-iminodiacetato-manganese(II)]

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Received 10 April 2006
Accepted 30 April 2006

In the title polymeric complex, $[Mn(C_4H_5NO_4)]_n$, the Mn^{II} ion assumes a distorted octahedral coordination, formed by four iminodiacetate (IDA) dianions. The tridentate IDA ligands chelate to the Mn atoms in a facial configuration and bridge Mn^{II} ions, forming a three-dimensional polymeric structure.

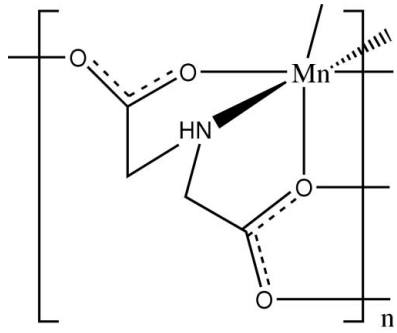
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.021
wR factor = 0.053
Data-to-parameter ratio = 13.5

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

Comment

The iminodiacetate (IDA) dianion has been used as a bridging ligand in the preparation of metal complexes (Yukawa, 1992; Liu & Xu, 2004). We present here the structure of a new Mn^{II} complex, (I), bridged by IDA.



(I)

The coordination environment around the Mn^{II} ion in the polymeric structure of (I) is shown in Fig. 1. The Mn^{II} ion is

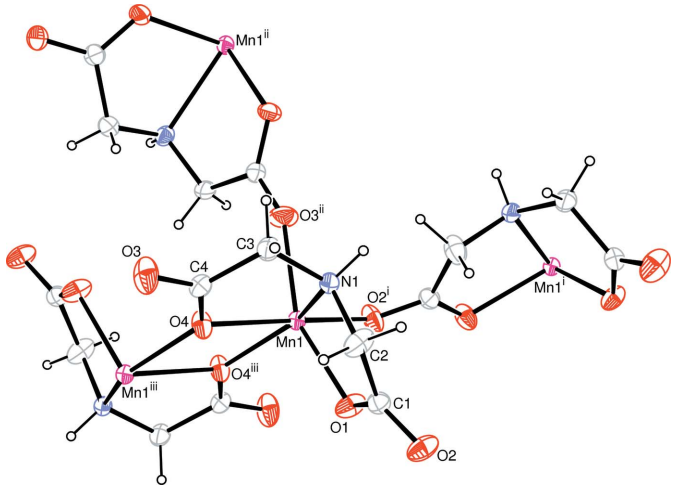


Figure 1
A segment of the polymeric structure of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). [Symmetry codes: (i) $\frac{1}{2}+x, y, \frac{1}{2}-z$; (ii) $\frac{1}{2}+x, \frac{1}{2}-y, 1-z$; (iii) $2-x, 1-y, 1-z$.]

located on a general position and assumes a distorted octahedral coordination (Table 1), formed by four IDA dianions. The tridentate IDA ligands chelate to the Mn^{II} ions in a facial configuration; one chelating five-membered ring is almost planar and the other adopts an envelope configuration. The carboxylate groups bridge the Mn^{II} ions, forming a three-dimensional polymeric structure.

Experimental

H_2IDA, $MnCl_2{\cdot}4H_2O$ and NaOH (molar ratio 1:1:1) were dissolved in a water/methanol solution (2:3, 25 ml). After stirring for 2 h at room temperature, the solution was sealed in a 40 ml Teflon-lined stainless steel vessel and heated at 453 K for 96 h under autogenous pressure. After cooling to room temperature, the resulting product of pale-pink rod-like crystals of (I) was filtered off (about 85% yield based on Mn). Elemental analysis calculated for $C_4H_5MnNO_4$: C 25.83, H 2.71, N 7.53%; found: C 25.42, H 2.96, N 7.24%.

Crystal data

$[Mn(C_4H_5NO_4)]$
M_r = 186.03
Orthorhombic, *Pbca*
a = 8.3923 (11) Å
b = 9.4570 (13) Å
c = 15.023 (2) Å
V = 1192.3 (3) Å^3
Z = 8
D_x = 2.073 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.16 mm^{-1}
T = 294 (2) K
Rod, pink
0.18 × 0.16 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.625, T_{max} = 0.775
6166 measured reflections
1226 independent reflections
1031 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.053
S = 1.04
1226 reflections
91 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0245P)^2 + 0.7854P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—N1	2.3042 (16)	Mn1—O3^{ii}	2.1424 (14)
Mn1—O1	2.1558 (14)	Mn1—O4	2.3014 (13)
Mn1—O2^{i}	2.1313 (14)	Mn1—O4^{iii}	2.1650 (13)

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

H atoms were placed in geometrically idealized positions, with C—H = 0.97 Å and N—H = 0.91 Å and refined in riding mode, with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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