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rac-Poly[bis(μ-tryptophanato)manganese(II)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.066
wR factor = 0.170
Data-to-parameter ratio = 12.1

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

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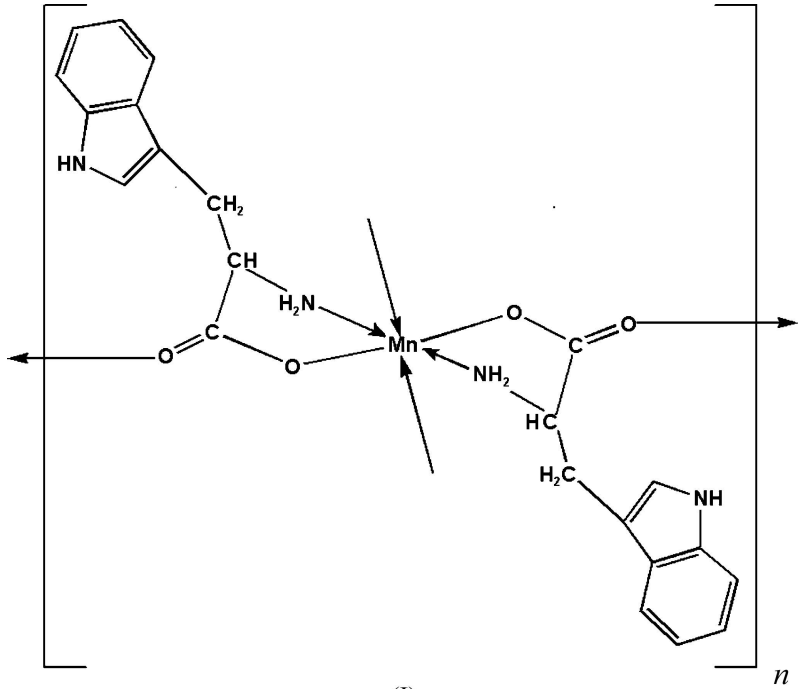
In the title compound, $[Mn(C_{11}H_{11}N_2O_2)_2]_n$, the Mn atom is chelated by the tryptophanate anion through the amino N and carboxylate O atoms; it is also linked to the carbonyl O atom of an adjacent monomer unit, forming a polymeric sheet. The Mn atom lies on an inversion centre.

Comment

Among coordination polymer frameworks based on molecules of biological interest (Waern & Harding, 2004) are some derived from amino acids. The title compound, (I), has a layer structure comprising tryptophanate anions and Mn ions. The structure is centrosymmetric. However, as the synthesis used an optically active reagent, racemization would have taken place under the reaction conditions. The Mn atom exists in an all-*trans* N_2O_4Mn octahedral coordination geometry; it is chelated by the anion through the amino N and carboxylate O atoms, and is coordinated by the carbonyl O atom of an adjacent monomer unit (Fig. 1). The manner in which adjacent units are connected gives rise to a layer structure (Fig. 2). The free NH group engages in an unimportant hydrogen-bonding interaction [N2—H2···O1($1-x, \frac{1}{2}+y, \frac{3}{2}-z$)].



(I)

Experimental

A mixture of $Mn(ClO_4)_2$ (0.023 g, 0.15 mmol), L-tryptophan (0.060 g, 0.30 mmol), pyridine (0.10 ml), methanol (0.40 ml) and water

(0.10 ml) was placed in a thick-walled Pyrex tube. The tube was frozen in liquid nitrogen and sealed under vacuum. It was heated at 393 K for 6 d. Plate-shaped crystals were then obtained. Elemental analysis found: C 57.24, H 4.88, N 12.28%; calcd: C 57.27, H 4.81, N 12.14%.

Crystal data

$[Mn(C_{11}H_{11}N_2O_2)_2]$	$Z = 2$
$M_r = 461.38$	$D_x = 1.520$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 19.874$ (4) Å	$\mu = 0.69$ mm^{-1}
$b = 5.3600$ (11) Å	$T = 293$ (2) K
$c = 9.5420$ (19) Å	Plate, colourless
$\beta = 97.41$ (3)°	0.30 × 0.30 × 0.10 mm
$V = 1008.0$ (4) Å^3	

Data collection

Siemens SMART CCD diffractometer	5347 measured reflections
	1728 independent reflections
φ and ω scans	1665 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)	$R_{int} = 0.056$
	$\theta_{max} = 25.0°$
$T_{min} = 0.819$, $T_{max} = 0.934$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.123P)^2 + 0.282P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.066$	
$wR(F^2) = 0.170$	
$S = 1.09$	$(\Delta/\sigma)_{max} < 0.001$
1728 reflections	$\Delta\rho_{max} = 0.74$ e Å^{-3}
143 parameters	$\Delta\rho_{min} = -0.65$ e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL97*
	Extinction coefficient: 0.22 (2)

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	2.1438 (16)	Mn1—N2	2.293 (2)
Mn1—O2	2.2186 (19)		
O1^i—Mn1—O2	91.64 (8)	O1—Mn1—N2^i	103.32 (7)
O1—Mn1—O2	88.36 (8)	C11—O1—Mn1	118.18 (15)
O1—Mn1—N2	76.68 (7)	C10—N2—Mn1	109.00 (15)
O2—Mn1—N2	88.28 (7)	C11^{ii}—O2—Mn1	127.31 (16)
O2^i—Mn1—N2	91.72 (7)		

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

Carbon-bound H atoms were constrained to ride on their parent atoms, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C). Nitrogen-bound H atoms were placed in calculated positions and constrained to ride on their parent atoms, with N—H = 0.86–0.90 Å and U_{iso}(H) = 1.2U_{eq}(N).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXTL*.

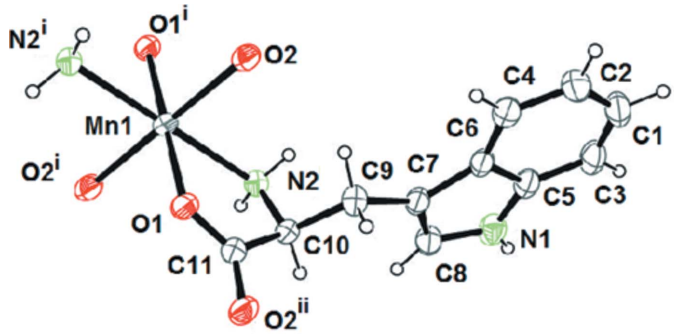


Figure 1
The coordination environment for (I), with non-H atoms shown as 30% probability ellipsoids. [Symmetry codes: (i) $-x, -y, -z$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.]

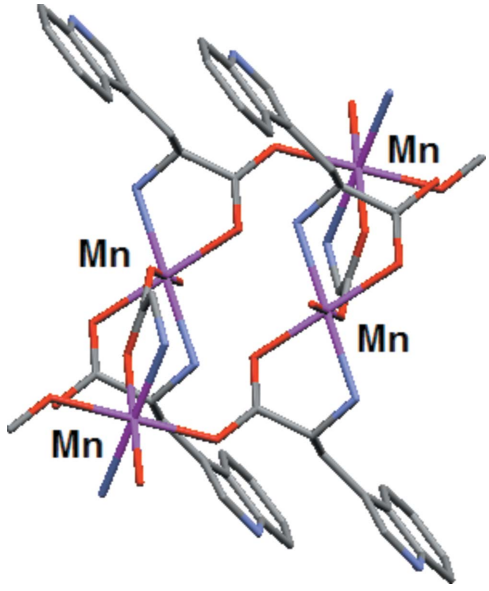


Figure 2
A segment of the two-dimensional structure. H atoms have been omitted.

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