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[*N*,*N*′-Bis(2-oxido-1-naphthylmethylidene)-propane-1,3-diamine]manganese(II)

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In the title mononuclear manganese(II) complex, $[Mn(C_{25}H_{20}N_2O_2)]$, the Mn atom and the central methylene group of the propanediamine fragment of the ligand lie on a mirror plane. The four-coordinate Mn atom binds to two N and two O atoms of the ligand, forming a square-planar geometry.

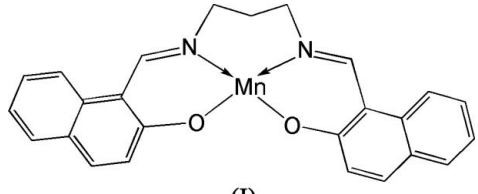
Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.007 Å
R factor = 0.046
wR factor = 0.122
Data-to-parameter ratio = 14.2

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

Comment

Manganese(II) compounds are very important in bioinorganic chemistry (Ciringh *et al.*, 1997; Chen *et al.*, 2003). The structure of a mononuclear manganese(II) complex, (I), is described here.



(I)

Atom Mn1 lies on a mirror plane, as does the methylene C13 and its substituent H atoms. Mn1 is four-coordinate, binding to two N and two O atoms of the ligand in a slightly distorted square-planar geometry (Fig. 1). The Mn—N and Mn—O bond lengths (Table 1) are comparable with the corresponding values observed in other manganese(II) complexes (Gallo, Solari, Re *et al.*, 1997; Gallo, Solari, Floriani *et al.*, 1997). The bond angles subtended by *cis* substituents on Mn1 range from 82.17 (19) to 94.3 (2)° (Table 1).

Experimental

Compound (I) was obtained by stirring propane-1,3-diamine (1.0 mmol, 79.2 mg), 2-hydroxy-1-naphthaldehyde (2.0 mmol, 343.5 mg) and manganese(II) acetate tetrahydrate (1.0 mmol, 245.1 mg) in EtOH solution (80 ml). The residue was recrystallized from an EtOH solution, giving brown block-like crystals.

Crystal data

$[Mn(C_{25}H_{20}N_2O_2)]$
M_r = 435.37
Orthorhombic, $Cmc2_1$
a = 30.650 (1) Å
b = 8.464 (3) Å
c = 7.769 (1) Å
V = 2015.5 (8) Å^3
Z = 4
D_x = 1.435 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1718 reflections
θ = 2.5–22.6°
μ = 0.68 mm^{-1}
T = 273 (2) K
Block, brown
0.32 × 0.28 × 0.22 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.812, T_{max} = 0.865
5125 measured reflections
1977 independent reflections
1541 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 26.5°
$h = -29 \rightarrow 38$
$k = -10 \rightarrow 10$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.122
S = 0.97
1977 reflections
139 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0679P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Absolute structure: Flack (1983), with 849 Friedel pairs
Flack parameter: −0.08 (4)

Table 1
Selected geometric parameters (Å, °).

Mn1—O1	1.842 (3)	Mn1—N1	1.867 (4)
O1^{i}—Mn1—O1	82.17 (19)	O1—Mn1—N1	91.75 (15)
O1^{i}—Mn1—N1	173.75 (14)	N1—Mn1—N1^{i}	94.3 (2)

Symmetry code: (i) $-x, y, z$.

All H atoms were constrained to their ideal geometries, with C—H = 0.93–0.97Å and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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*.

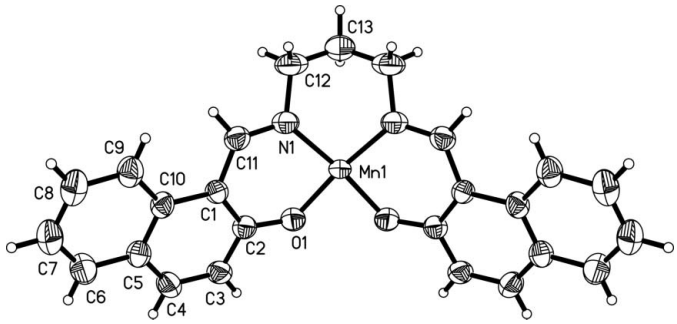


Figure 1
The structure of (I), showing the atom-numbering scheme, with displacement ellipsoids drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operator $(-x, y, z)$.

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