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[1,2-Diphenyl-*N*,*N*′-bis(salicylidene)-(*RR*,*SS*)-1,2-ethanediyldiaminato]-nitridomanganese(V)

Hirofumi Iwamoto, Masanobu Tsuchimoto and Shigeru Ohba*

Department of Chemistry, Faculty of Science and Technology, Keio University, Hiyoshi 3-14-1, Kohoku-ku, Yokohama 223-8522, Japan
Correspondence e-mail: ohba@chem.keio.ac.jp

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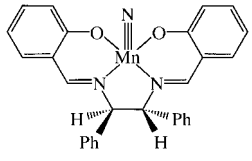
The title compound, [MnN($C_{28}H_{22}N_2O_2$)], has a distorted square-pyramidal coordination with an Mn≡N bond length of 1.516 (2) Å at the apical position. The five-membered chelate ring adopts a *gauche* conformation with the two phenyl groups in equatorial orientations.

Comment

The crystal structure of [MnN{sal-(*SS*)-stien}]·CH_3CN was reported by Chang *et al.* (1998). We report here the crystal structure of [MnN(sal-*rac*-stien)], (I).



(I)

Experimental

The title compound, [MnN(sal-*rac*-stien)], was prepared under aerobic conditions by the reaction of the chloromanganese(III) complex [MnCl(sal-*rac*-stien)] with NH_4OH (15 equivalents) and NaOCl (6 equivalents). Crystals were grown from an acetonitorile solution.

Crystal data

[MnN($C_{28}H_{22}N_2O_2$)]
M_r = 487.44
Triclinic, $P\overline{1}$
a = 10.124 (4) Å
b = 12.672 (3) Å
c = 9.632 (2) Å
α = 110.83 (2)°
β = 96.36 (3)°
γ = 85.32 (3)°
V = 1146.6 (6) Å^3
Z = 2
D_x = 1.412 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 14.7–15.0°
μ = 0.607 mm^{-1}
T = 298 K
Prismatic, green
0.7 × 0.2 × 0.2 mm

Data collection

Rigaku AFC-7*R* diffractometer
θ–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.824, T_{max} = 0.886
5556 measured reflections
5258 independent reflections
4696 reflections with $I > 2\sigma(I)$
R_{int} = 0.007
θ_{max} = 27.5°
$h = -13 \rightarrow 0$
$k = -16 \rightarrow 16$
$l = -12 \rightarrow 12$
3 standard reflections
every 150 reflections
intensity decay: none

Refinement

Refinement on F^2
$R(F)$ = 0.033
$wR(F^2)$ = 0.090
S = 1.04
4696 reflections
307 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2 + 0.5302P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å).

Mn1—O2	1.908 (1)	Mn1—N5	1.956 (1)
Mn1—O3	1.908 (1)	Mn1—N6	1.516 (2)
Mn1—N4	1.962 (1)		

All H-atom positional parameters were calculated geometrically and fixed with U_{iso}(H) = 1.2U_{eq}(parent atom).

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1993); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *TEXSAN*.

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