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## Key indicators

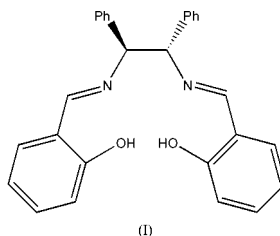
Single-crystal X-ray study  
 $T = 173$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.042  
 $wR$  factor = 0.117  
Data-to-parameter ratio = 10.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**(-)-(1*S*,2*S*)-*N,N'*-Bis(salicylidene)-1,2-diphenyl-1,2-ethanediamine**

The crystal structure of the title compound,  $(-)-2,2'-[(1*S*,2*S*)-1,2\text{-diphenyl-1,2-ethanediylbis(nitrilomethylidene)]\text{diphenol}$ ,  $\text{C}_{28}\text{H}_{24}\text{N}_2\text{O}_2$ , has been determined at 173 (2) K in the non-centrosymmetric space group  $P2_12_12$ . The molecule lies on a crystallographic twofold axis of symmetry. The asymmetric unit contains one-half of the molecule. An intramolecular O—H $\cdots$ N hydrogen bond is formed between the phenol OH group and the Schiff base N atom.

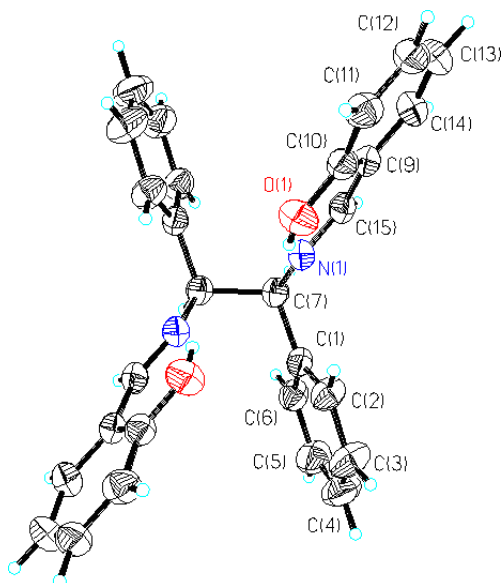
Received 13 August 2003  
Accepted 5 September 2003  
Online 18 September 2003

## Comment

Manganese–salen complexes are actively used as catalysts owing to their ability to highly stereoselectively epoxidize unfunctionalized alkenes (Lane & Burgess, 2003). Schiff base (I) was a precursor to one of the first manganese–Schiff base asymmetric epoxidation catalysts developed by Jacobsen and coworkers (Zhang *et al.*, 1990). The structure of *N,N'*-disalicylidene-*meso*-(*R,S*)-1,2-diphenylethylenediamine was determined by Senn & Nowacki (1977). Here we report the crystal structure of the pure (*S,S*) enantiomer of (I).



Compound (I) was obtained by a simple Schiff base condensation of salicylaldehyde and (1*S*,2*S*)-(-)-1,2-diphenyl-1,2-ethanediamine. It crystallizes in the non-centrosymmetric space group  $P2_12_12$ . The molecule lies on a crystallographic twofold axis of symmetry, so only one-half of the molecule constitutes the asymmetric unit (Fig. 1). As in the case of the *meso* compound, the structure is stabilized by the formation of an intramolecular hydrogen bond between the phenol OH group and the Schiff base N atom, such that a six-membered ring is formed. The angle between the planes defined by the rings of the salicylidene fragment and the phenyl substituent in compound (I) is  $63.76(6)^\circ$ , compared to just  $23.8^\circ$  in the *meso* isomer. Unlike those in the *meso* compound, which possesses a center of inversion, the planes formed by the symmetry-related benzene rings are not parallel in (I). The angles between the corresponding planes are  $29.60(6)^\circ$  for the phenyl rings and  $35.55(7)^\circ$  for the salicylidene benzene rings. A packing diagram of (I) is presented in Fig. 2.



**Figure 1**  
View of the molecule of (I), showing the atom-labeling scheme in the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level.

## Experimental

The title compound was prepared according to the general procedure of Jacobsen (Zhang *et al.*, 1990). (1*S*,2*S*)-(–)-1,2-Diphenyl-1,2-ethanediamine (99% purity, 99% e.e.) and salicylaldehyde were purchased from Acros and used without further purification. Suitable crystals were obtained by slow evaporation of an ethanol solution of (I). Spectroscopic analysis:  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , p.p.m.):  $\delta$  13.3 (*br*, 2H), 8.35 (*s*, 2H), 7.35–7.15 (*m*, 14H), 6.99 (*d*, 2H,  $J = 11.5$  Hz), 6.84 (*t*, 2H,  $J = 11.5$  Hz), 4.78 (*s*, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , p.p.m.):  $\delta$  166.4, 161.1, 139.6, 132.8, 132.0, 128.6, 128.1, 127.8, 119.0, 118.8, 117.1, 80.4;

### Crystal data

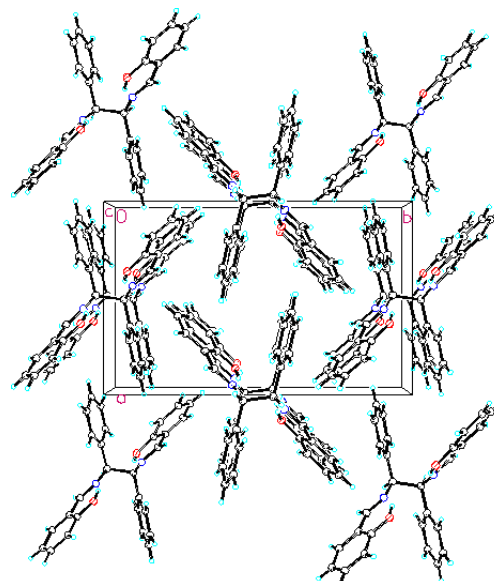
$\text{C}_{28}\text{H}_{24}\text{N}_2\text{O}_2$	Mo $K\alpha$ radiation
$M_r = 420.49$	Cell parameters from 6042 reflections
Orthorhombic, $P2_12_12$	$\theta = 2.4\text{--}28.2^\circ$
$a = 10.1341$ (13) Å	$\mu = 0.08$ mm $^{-1}$
$b = 16.168$ (2) Å	$T = 173$ (2) K
$c = 6.9249$ (9) Å	Block, yellow
$V = 1134.6$ (3) Å $^3$	$0.40 \times 0.22 \times 0.15$ mm
$Z = 2$	
$D_x = 1.231$ Mg m $^{-3}$	

### Data collection

Bruker SMART CCD area-detector diffractometer	1605 independent reflections
$\varphi$ and $\omega$ scans	1439 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.041$
$T_{\text{min}} = 0.970$ , $T_{\text{max}} = 0.988$	$\theta_{\text{max}} = 28.3^\circ$
7362 measured reflections	$h = -13 \rightarrow 12$
	$k = -20 \rightarrow 21$
	$l = -9 \rightarrow 9$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0645P)^2 + 0.1064P]$
$R[F^2 > 2\sigma(F^2)] = 0.042$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.117$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.09$	$\Delta\rho_{\text{max}} = 0.18$ e Å $^{-3}$
1605 reflections	$\Delta\rho_{\text{min}} = -0.17$ e Å $^{-3}$
150 parameters	Extinction correction: SHELXL97
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.079 (9)



**Figure 2**  
The molecular packing of (I), viewed along the  $c$  axis.

**Table 1**

Selected geometric parameters (Å, °).

O1—C10	1.348 (2)	C1—C7	1.517 (2)
N1—C15	1.270 (2)	C7—C7 <sup>i</sup>	1.559 (3)
N1—C7	1.453 (2)	C9—C15	1.449 (2)
C15—N1—C7	119.26 (14)	O1—C10—C9	120.93 (15)
N1—C7—C1	111.64 (13)	N1—C15—C9	121.70 (15)

Symmetry codes: (i)  $-x, 1 - y, z$ .

**Table 2**

Hydrogen-bonding geometry (Å, °).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
O1—H1 $\cdots$ N1	1.03 (4)	1.61 (4)	2.5566 (19)	151 (3)

Carbon-bound H atoms were placed in idealized positions ( $\text{C--H} = 0.95\text{--}1.0$  Å) and refined using a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The H atom bound to the phenol O atom was found in a difference Fourier map and refined isotropically. Friedel pairs have been merged and not used as independent data. The absolute configuration was established by reference to the chiral center in the synthetic procedure.

Data collection: SMART (Bruker, 1998); cell refinement: SMART; data reduction: SAINT (Bruker, 1998); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2000); software used to prepare material for publication: XCIF in SHELXTL.

The CCD-based X-ray diffractometer at Tufts University was purchased through Air Force DURIP Grant F49620-01-1-0242.

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