

[*N,N'*-Bis(salicylidene)-1,2-diphenyl-(*RS,SR*)-1,2-ethanediaminato]-nickel(II)

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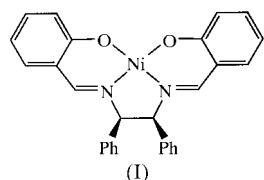
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In crystals of the title compound, $[\text{Ni}(\text{C}_{28}\text{H}_{22}\text{N}_2\text{O}_2)]$, the coordination geometry around the Ni atom is square planar with a slight tetrahedral distortion. The five-membered *N,N'*-chelate ring adopts a distorted *gauche* conformation with the two phenyl groups in axial and equatorial orientations.

Comment

The thermal dehydrogenation reaction of $[\text{Ni}(3\text{-EtOsal}-meso-stien)]$ with $[\text{VO}(\text{salen})]\text{NO}_3$ in the solid state has been



investigated by Hoshina *et al.* (2000), where $\text{H}_2(3\text{-EtOsal}-meso-stien)$ is *N,N'*-bis(3-ethoxysalicylidene)-1,2-diphenyl-1,2-ethanediamine. The crystal structure of $[\text{Ni}(\text{sal-meso-stien})]$, (I), is presented here, where *sal-meso-stien* is *N,N'*-bis(salicylidene)-1,2-diphenyl-1,2-ethanediamine.

Experimental

The title complex, $[\text{Ni}(\text{sal-meso-stien})]$, was prepared by the reaction of a hot methanol solution (30 ml) of nickel(II) acetate tetrahydrate (0.249 g, 1 mmol) with the Schiff base ligand $\text{H}_2(\text{sal-meso-stien})$ (0.421 g, 1 mmol). The resulting red-brown precipitate was collected by filtration and washed with ether (yield 90%). The red crystals of $[\text{Ni}(\text{sal-meso-stien})]$ were grown by slow evaporation of an acetonitrile solution.

Crystal data

$[\text{Ni}(\text{C}_{28}\text{H}_{22}\text{N}_2\text{O}_2)]$	$D_x = 1.402 \text{ Mg m}^{-3}$
$M_r = 477.19$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 25 reflections
$a = 12.517 (2) \text{ \AA}$	$\theta = 14.2\text{--}14.9^\circ$
$b = 11.500 (3) \text{ \AA}$	$\mu = 0.887 \text{ mm}^{-1}$
$c = 16.413 (2) \text{ \AA}$	$T = 297 \text{ K}$
$\beta = 106.893 (9)^\circ$	Prismatic, red
$V = 2260.7 (6) \text{ \AA}^3$	$0.5 \times 0.4 \times 0.3 \text{ mm}$
$Z = 4$	

Data collection

Rigaku AFC-5 diffractometer	$R_{\text{int}} = 0.026$
θ - 2θ scans	$\theta_{\text{max}} = 27.5^\circ$
Absorption correction: ψ scan (North <i>et al.</i> , 1968)	$h = 0 \rightarrow 16$
$T_{\text{min}} = 0.658$, $T_{\text{max}} = 0.766$	$k = 0 \rightarrow 14$
5415 measured reflections	$l = -21 \rightarrow 21$
5182 independent reflections	3 standard reflections
3469 reflections with $I > 2\sigma(I)$	every 100 reflections
	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.2639P]$
$R(F) = 0.044$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.109$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.47 \text{ e \AA}^{-3}$
3469 reflections	$\Delta\rho_{\text{min}} = -0.28 \text{ e \AA}^{-3}$
298 parameters	H-atom parameters not refined

Table 1
Selected geometric parameters (\AA , $^\circ$).

Ni—O2	1.846 (2)	Ni—N4	1.848 (2)
Ni—O3	1.840 (2)	Ni—N5	1.855 (2)
O2—Ni—O3	84.49 (8)	O3—Ni—N4	174.53 (10)
O2—Ni—N4	94.70 (9)	O3—Ni—N5	94.85 (9)
O2—Ni—N5	171.6 (1)	N4—Ni—N5	86.74 (10)

All H-atom positions were calculated geometrically and fixed with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$.

Data collection and cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); software used to prepare material for publication: *TEXSAN*.

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