

## Thiosemicarbazone Complexes of Phenylmercury(II): Synthesis and Spectral Characterization

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### Structured Abstract:

**Purpose:** To synthesize and characterize two N,S donor Schiff base ligands and their complexes with phenylmercury(II) acetate.

**Methods:** Condensation of thiosemicarbazide with 2-hydroxyacetophenone and diacetylmonooxime yielded two N, S donor Schiff base ligands Haptsc and Hdmtsc. The reaction of phenylmercury(II) acetate with these Schiff base ligands has produced two new light-yellow coloured phenylmercury(II) complexes [PhHg(aptsc)] (**1**) and [PhHg(dmtsc)] (**2**). The physicochemical techniques e.g. elemental analyses, spectroscopic methods (IR, Electronic, NMR) and conductivity measurements have been applied to characterize the ligands and the newly synthesized complexes.

**Findings:** Based on the experimental data and on comparison with other related compounds both the Schiff base ligands are found to behave in a monobasic fashion and the corresponding complexes may be proposed to adopt Y-shaped geometry around mercury(II) by phenyl carbon, thiol sulphur and azomethine nitrogen atom.

**Originality:** The thione and thiol form of the ligands may remain in equilibrium in solution through enethiolization process and the bonding with the phenylmercury(II) ion has been observed to take place through thiol form of sulphur.

**Keywords:** Schiff Base, Phenylmercury(II), Spectroscopy, NS Donor.

**Paper Type:** Research Note.

### Introduction

The chemistry of (N, S, O) donor Schiff base ligands and their corresponding metal complexes has been gaining considerable interest for their interesting and important properties, e.g., their fascinating structural diversities (Dhar *et al.*, 2005; Vyas *et al.*, 2011; Thomas *et al.*, 2004; Sarkar *et al.*, 2005), catalytic activities in a number of organic transformations and other reactions (Prakash *et al.*, 2011; Temel *et al.*, 2012; Kathale *et al.*, 2001), ability to be used as magnetic materials (Andruh *et al.*, 2011; Miyasaka *et al.*, 1996;

Costes *et al.*, 2002) and photo-induced chemical behavior (Trujillo *et al.*, 2010; Cozzi *et al.*, 2003). The biological activities of metal complexes involving such thiosemicarbazone Schiff base ligands have also been widely studied (Belicchi-Ferrari *et al.*, 2005; Ali *et al.*, 2002; Jayabalakrishnan *et al.*, 2001; Al-Amiery *et al.*, 2012; Rodriguez-Argüelles *et al.*, 1995). The antibacterial, anti-tumoral, antiviral, antimalarial and anti-tuberculosis activities are effectively shown by them (Raman *et al.*, 2001; Parashar *et al.*, 1988; da Silva *et al.*, 2011; Neelakantan *et al.*, 2010). The large size and  $d^{10}$  configuration of mercury(II) make it different from other transition elements in their coordination chemistry with (N, S, O) donor systems (Montazerzohori *et al.*, 2009; Gupta *et al.*, 2007; Donia *et al.*, 2008). Mercury is noted as one of the most toxic heavy metals on earth and toxicity of mercury depends on the various occurring forms. Organo-mercury compounds are found to be more toxic than elemental mercury and other inorganic mercury compounds (Boening, 2000; Hempel *et al.*, 1995; Clarkson *et al.*, 1997).

The study of organomercury(II)-thione complexes find their natural importance due to its great similarity with the methylmercury(II) cation and its activity for bio-methylation process. Such organomercury(II) moiety strongly interacts with the sulphur atoms present in the cysteinyl groups of polypeptides. In such complexes, mercury(II) ion primarily binds with sulphur atom due to soft-soft interaction and such bond formation reinforces the other atoms like nitrogen or oxygen to create a secondary interaction with the mercury(II) cation. High complexing ability and chelation property make such (N, S, O) donor Schiff base ligands to be effectively used as scavengers for some toxic metals like, Cd, Hg etc.

In this presentation we have studied the synthesis and characterization of two (N, S) donor Schiff base ligands Haptsc and Hdmtsc and their reactions with phenylmercury(II) acetate.

## **Experimental**

### ***Materials***

All chemicals user were of AR grade and solvents were purified and dried before use. Phenylmercury(II) acetate (Aldrich, Germany) was used as received.

**Synthesis of ligand (Haptsc):** 2-hydroxyacetophenone (0.70 g, 5 mmol) was taken in methanol (10 ml) to which thiosemicarbazide (0.47 g, 5 mmol) taken in methanol (10 ml) was added dropwise with stirring. Immediately a yellow solution was obtained. Glacial acetic acid (3/4 drops) was then added to it with stirring to facilitate the condensation reaction and stirring continued for 3 h at room temperature. The yellow solution on slow evaporation gave light yellow micro-crystals of Haptsc.

**Synthesis of ligand (Hdmtsc):** Diacetylmonoxime (0.52 g, 5 mmol) was dissolved in methanol (10 ml) and thiosemicarbazide (0.47 g, 5 mmol) taken methanol (10 ml) was then added to it and the mixture turns very light yellow in colour. Glacial acetic acid (3/4 drops) was then added to it and the mixture was stirred for 2 h at room temperature. Thereafter, the light yellow solution was refluxed at water bath for two hours. Light yellow micro-crystals of Hdmtsc were grown after concentration and slow evaporation.

**Synthesis of [PhHg(aptsc)] (1):** A suspension of phenylmercury(II) acetate (1.68 g, 5 mmol) was prepared by dissolving it in dry ethanol (25 ml) and filtered directly into a methanolic solution (10 ml) of the ligand, Haptsc (1.05 g, 5 mmol). The mixture was heated under gentle reflux for about an hour and filtered while hot. The filtrate, on concentration and cooling, yielded a light yellowish compound.

**Synthesis of [PhHg(dmtsc)] (2):** A suspension of phenylmercury(II) acetate (1.68 g, 5 mmol) was prepared by dissolving it in dry ethanol (25 ml) and filtered directly into a methanolic solution (10 ml) of the ligand, Hdmtsc (0.87 g, 5 mmol). The mixture was heated under gentle reflux for about an hour and filtered while hot. The filtrate, on concentration and cooling, yielded a light yellowish compound.

### **Physical Measurements**

Elemental analyses were carried out at the Regional Sophisticated Instrumentation Center, Central Drug Research Institute, Lucknow, India. The electronic spectra were recorded (in  $10^{-5}$  M  $\text{CHCl}_3$  solution) using a Simadzu UV-1601 spectrophotometer and Emission spectra were recorded in Perkin–Elmer L52 spectrophotometer using  $10^{-5}$  M  $\text{CHCl}_3$  solution at room temperature. Infrared spectral data were collected (KBr pellets) using a Perkin–Elmer L120-000A spectrophotometer and  $^1\text{H}$  NMR spectra of the samples were measured in  $\text{DMSO}-d_6$  at the Indian Institute of Chemical Biology, Kolkata, West Bengal, India using a Bruker-400 MHz instrument at room temperature.

## **Results and Discussion:**

### **Syntheses**

The reactions of 2-hydroxy acetophenone and diacetylmonoxime with thiosemicarbazide in 1:1 molar ratio in methanol yielded the (N, S, O) donor thiosemicarbazone ligands (Haptsc and Hdmtsc) (Fig. 1). Both the ligands have a proton adjacent to the thione group. The thione group is relatively unstable in the monomeric form and tends to turn to the more stable C-S bond by enethiolization if there is at least one proton adjacent to thione group (Mayer, 1967). Therefore, the thione and the thiol may remain in equilibrium in solution (Fig. 2) and the ligands behave in a monobasic bidentate fashion; bonding through N and S atoms with the mercury ions.

The treatment of phenylmercury(II) acetate with 2-hydroxy acetophenone thiosemicarbazone (Haptsc) and diacetylmonoxime thiosemicarbazone (Hdmtsc) in dry ethanol under gentle refluxing conditions resulted light yellow complexes [PhHg(aptsc)] (1) and [PhHg(dmtsc)] (2) (Scheme 1). These two complexes are generally soluble in DMSO, acetonitrile and nitromethane, and partially soluble in acetone and chloroform. The isolated metal complexes (1) and (2) are stable at room temperature and have been characterized by elemental analyses, molar conductance values, magnetic moments and spectroscopic (IR, <sup>1</sup>H NMR and UV-Vis) data. Some of the characterization data are shown in Table 1.

### **Molar conductance and Magnetic Moments**

The molar conductance values (Table 1) of the complexes (1) and (2) in DMSO are found as 8.6 and 10.2  $\Omega^{-1} \text{ cm}^2 \text{ mol}^{-1}$  respectively suggesting the non-electrolytic nature of both the complexes (Geary, 1971). The magnetic susceptibilities of the complexes under investigation were measured in the solid state at room temperature and found to be diamagnetic in nature.

### **Infrared and <sup>1</sup>H NMR Spectra:**

The infrared spectra of the free ligands Haptsc and Hdmtsc in solid state do not show any  $\nu_{\text{SH}}$  bands at  $\sim 2600 \text{ cm}^{-1}$  (Dey *et al.*, 2006; Dey *et al.*, 2006; Colthup *et al.*, 1964; Casas *et al.*, 1993), but instead an intense band for  $\nu_{\text{C=S}}$  at  $920 \text{ cm}^{-1}$  and  $880 \text{ cm}^{-1}$  are observed for Haptsc and Hdmtsc respectively. This  $\nu_{\text{C=S}}$  band disappears in the complexes and a new band around  $770$  and  $780 \text{ cm}^{-1}$  is observed for Haptsc and Hdmtsc respectively due to  $\nu_{\text{C-S}}$

suggesting mercury coordination through thiol sulfur. This mode is further supported by the presence of a medium band around  $340\text{ cm}^{-1}$  and  $350\text{ cm}^{-1}$  in case of Haptsc and Hdmtsc respectively assignable to  $\nu\text{Hg-S}$ . The bands due to  $\nu\text{NH}$  of the free ligands are located in the region  $3300$  and  $3250\text{ cm}^{-1}$ , but the  $\nu\text{OH}$  band at  $3500\text{ cm}^{-1}$  is not observed possibly due to strong hydrogen bonding which causes a shift to a lower frequency. Moreover, the  $\nu\text{C=N}$  stretching mode is observed at a slightly lower wave number in both the complexes suggesting the coordination of this C=N with phenylmercury. These observations for the two complexes suggest a similar type of N,S coordination mode for both the complexes. The representative infrared spectra of the Schiff base ligand (Haptsc) is shown below (Fig. 3).

The bands at  $1562$  (sh),  $1476$  (m),  $1005$  (m),  $989$  (m),  $716$  (vs),  $444$  (s),  $232$  (s) and  $184$  (sh) for both of these complexes are characteristic of a phenylmercury ring (Dey *et al.*, 2006; Colthup *et al.*, 1964; Casas *et al.*, 1993; Sarkar *et al.*, 2007).

The  $^1\text{H}$  NMR spectra for the ligands Haptsc and Hdmtsc show chemical shift due to a NH proton in  $\text{CDCl}_3$  at  $7.2$  and  $7.1$  ppm respectively which were disappeared in the two phenylmercury(II) complexes. The phenolic  $-\text{OH}$  signals of the Haptsc at  $4.8$  ppm shifts to lower field for complex (1) at  $4.6$  ppm, but there is no deprotonation. This is observed possibly due to strong hydrogen bonding. The oxime  $-\text{OH}$  signals of Hdmtsc shows a similar shifting to lower field in complex (2). Thus both the ligands coordinate to the phenylmercury(II) as monobasic ligands. The phenyl ring proton signals appear in the range  $6.6$ – $7.8$  ppm for the ligand Haptsc as well as both complexes. The methyl protons of Haptsc and complex (1) are observed at  $1.5$  and  $1.6$  ppm respectively. While signals of the methyl protons are observed for Hdmtsc and complex (2) at  $1.6$ – $1.9$  ppm. The chemical shifts of the free  $\text{NH}_2$  (2H) in both the ligands and complexes are observed at  $2.1$ – $2.3$  ppm (Dey *et al.*, 2006; Dey *et al.*, 2006; Colthup *et al.*, 1964; Casas *et al.*, 1993; Sarkar *et al.*, 2007).

### **Electronic Spectra:**

The free ligand Haptsc shows absorption bands at  $259$ ,  $346$  and  $474$  nm and Hdmtsc shows absorption bands (Fig. 4) at  $252$ ,  $343$  and  $467$  nm. The bands in the region  $343$ – $346$  nm and  $252$ – $259$  nm may be due to  $n-\pi^*$  and  $\pi-\pi^*$  transitions, respectively (Colthup *et al.*, 1964; Syamal *et al.*, 1981). The absorption bands are observed at slightly shifted position for the phenylmercury(II) complexes. The dependence of the solution absorption spectra on original Schiff bases suggests that the transitions are mainly ligand-centered transitions. Therefore,

the electronic absorption spectra are probably dominated by intraligand  $\pi-\pi^*$  transitions possibly mixed with a small contribution from the metal in the HOMO and the LUMO (Wong *et al.*, 2004).

### **Conclusion**

Two thiosemicarbazone ligands, 2-hydroxy acetophenone thiosemicarbazone (Haptsc) and diacetylmonoxime thiosemicarbazone (Hdmtsc) have been synthesized and characterized. In solution the 'thione' form of the ligands remain in equilibrium with its 'thiol' form. Both the ligands have been found to behave in a monobasic bidentate fashion on reaction with the phenylmercury ion to produce the complexes having Y-shaped geometry around mercury(II).

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**Table 1: Some characterization data of the complexes**

Sl. No.	Compound	Colour	Analyses Found (Calcd.) (%)				$\Lambda_M^a$ ( $\Omega^{-1}$ $\text{cm}^2\text{mol}^{-1}$ )	$\mu_{\text{eff}}^b$ B.M
			C	H	N	S		
1	Haptsc $\text{C}_{19}\text{H}_{11}\text{N}_3\text{OS}$	Yellow	50.82 (51.65)	5.10 (5.29)	20.26 (20.07)	15.05 (15.32)	–	–
2	Hdmtsc $\text{C}_5\text{H}_{10}\text{N}_5\text{OS}$	Yellow	34.21 (34.46)	5.65 (5.78)	32.55 (32.15)	18.06 (18.40)	–	–
3	[PhHg(aptsc)] (1) $\text{C}_{15}\text{H}_{16}\text{HgN}_3\text{OS}$	Yellow	36.46 (36.99)	3.06 (3.32)	8.15 (8.62)	5.99 (6.58)	8.6	Dia <sup>c</sup>
4	[PhHg(dmtsc)] (2) $\text{C}_{11}\text{H}_{15}\text{HgN}_4\text{OS}$	Yellow	28.96 (29.26)	3.01 (3.35)	12.01 (12.42)	6.86 (7.11)	10.2	Dia <sup>c</sup>

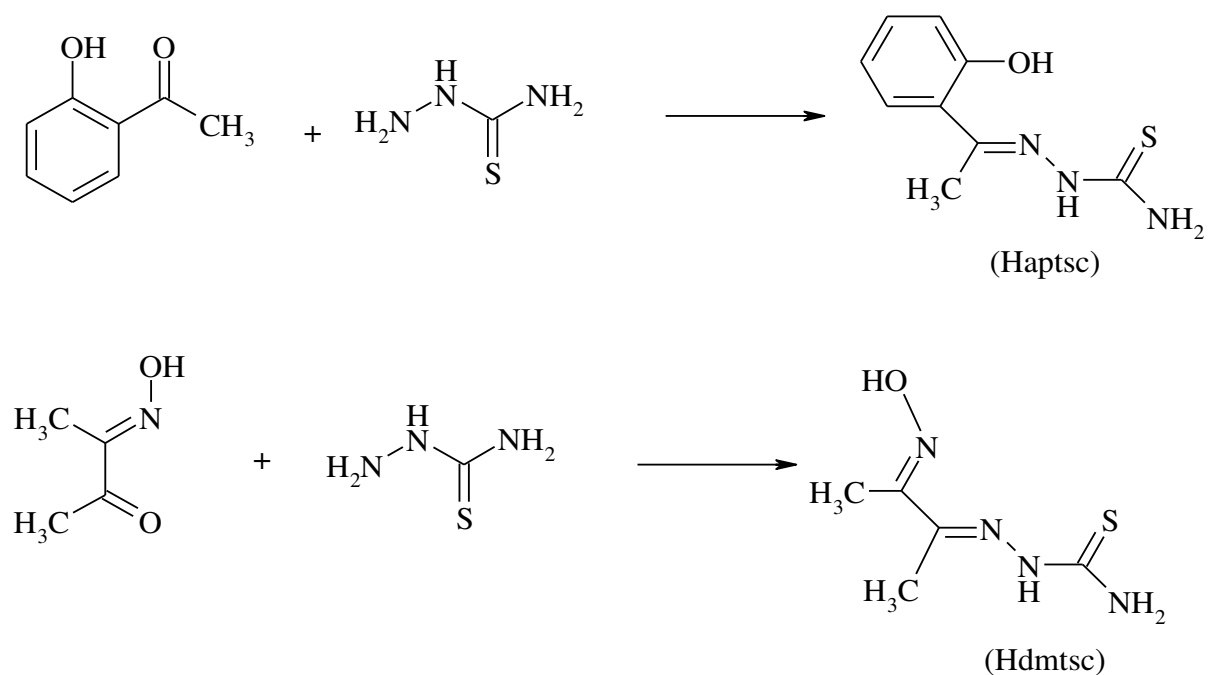
a) Solid state at room temperature, b)  $10^{-3}$  M solution in DMSO at room temperature, c) Diamagnetic

**Table 2: Infrared Spectral data of the ligands and complexes**

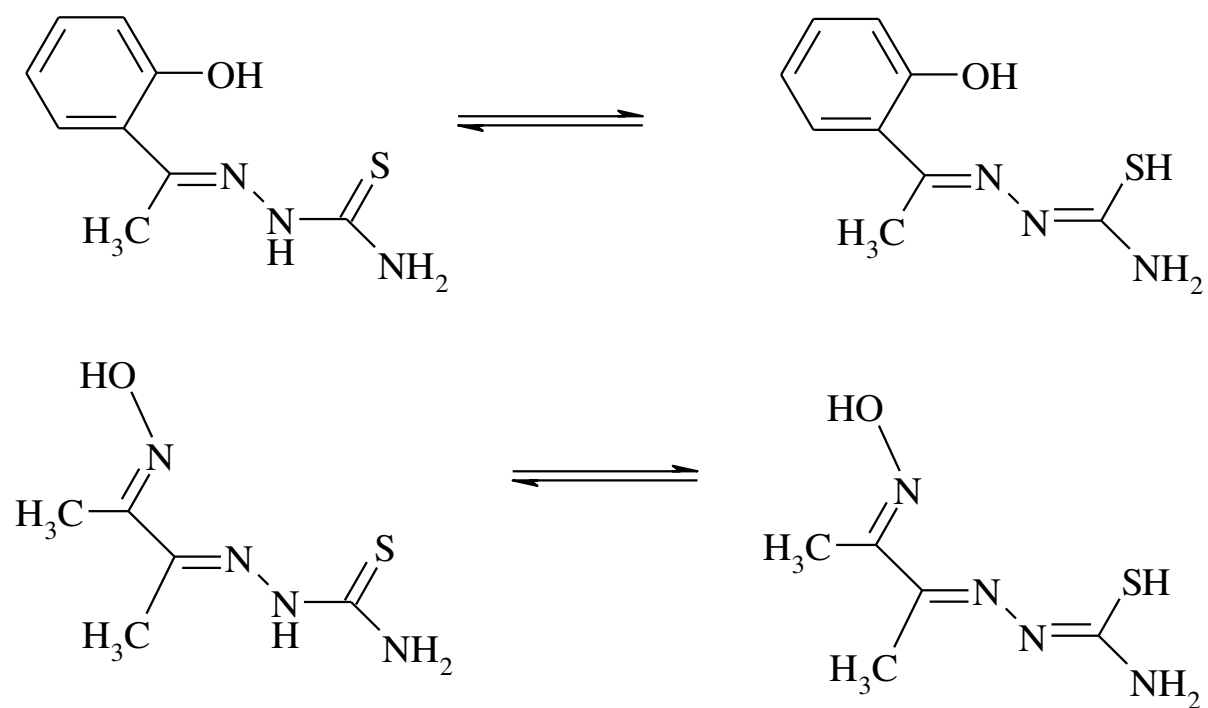
Ligand / Complex	$\nu_{\text{C=N}}$ ( $\text{cm}^{-1}$ )	$\nu_{\text{C=S}}$ ( $\text{cm}^{-1}$ )	$\nu_{\text{C-S}}$ ( $\text{cm}^{-1}$ )	$\nu_{\text{N-H}}$ ( $\text{cm}^{-1}$ )	$\nu_{\text{Hg-S}}$ ( $\text{cm}^{-1}$ )
Haptsc	1610	920	-	3300 (br)	-
Hdmtsc	1605	880	-	3250 (br)	-
[PhHg(aptsc)] (1)	1590	-	770	3300 (br)	340
[PhHg(dmtsc)] (2)	1580	-	780	3200 (br)	350

**Table 3: NMR Spectral data ( $\delta$  values in ppm) of the ligands and complexes**

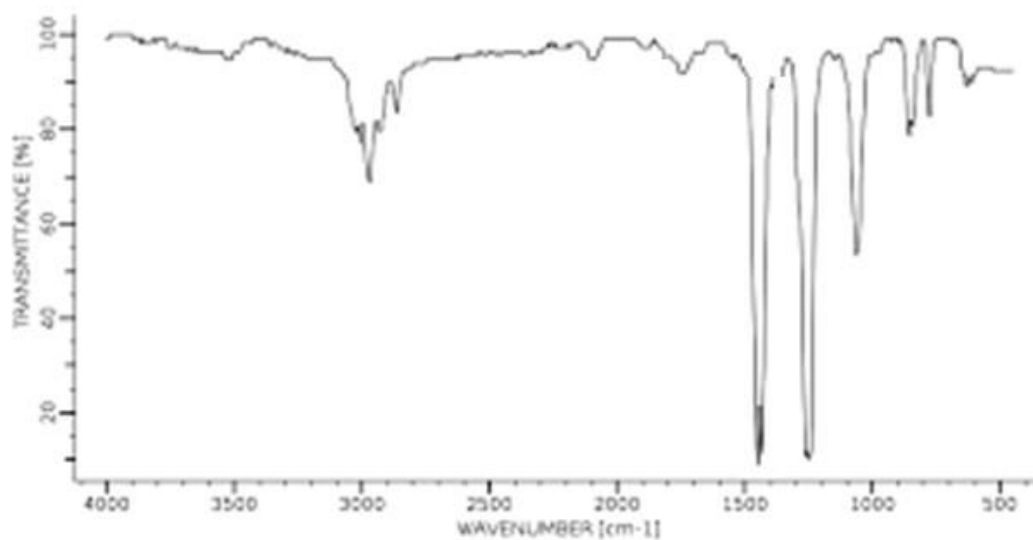
Ligand / Complex	-OH	-CH <sub>3</sub>	-NH	-NH <sub>2</sub>	-C <sub>6</sub> H <sub>4</sub> / -C <sub>6</sub> H <sub>5</sub>
Haptsc	4.8	1.5	7.2	2.1	6.6-7.8
Hdmtsc	2.1	1.8, 1.6	7.1	2.2	-
[PhHg(aptsc)] (1)	4.6	1.6	-	2.3	6.8-7.7
[PhHg(dmtsc)] (2)	2.0	1.9, 1.7	-	2.1	6.9-7.6



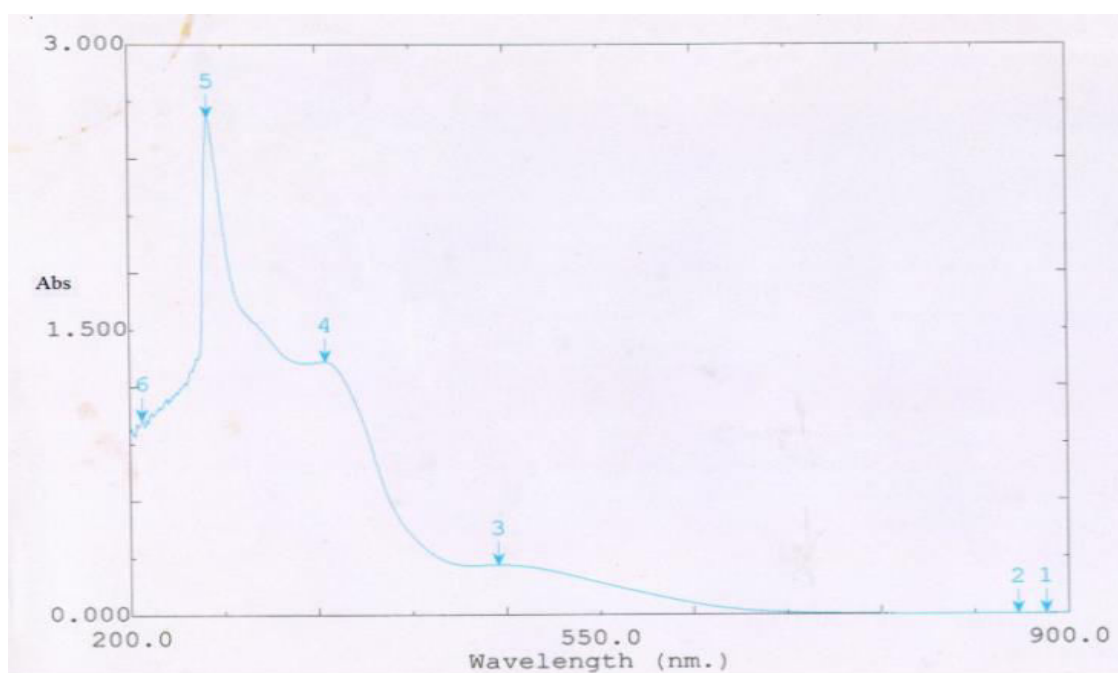
**Figure-1:** Formation of Schiff Base Ligands



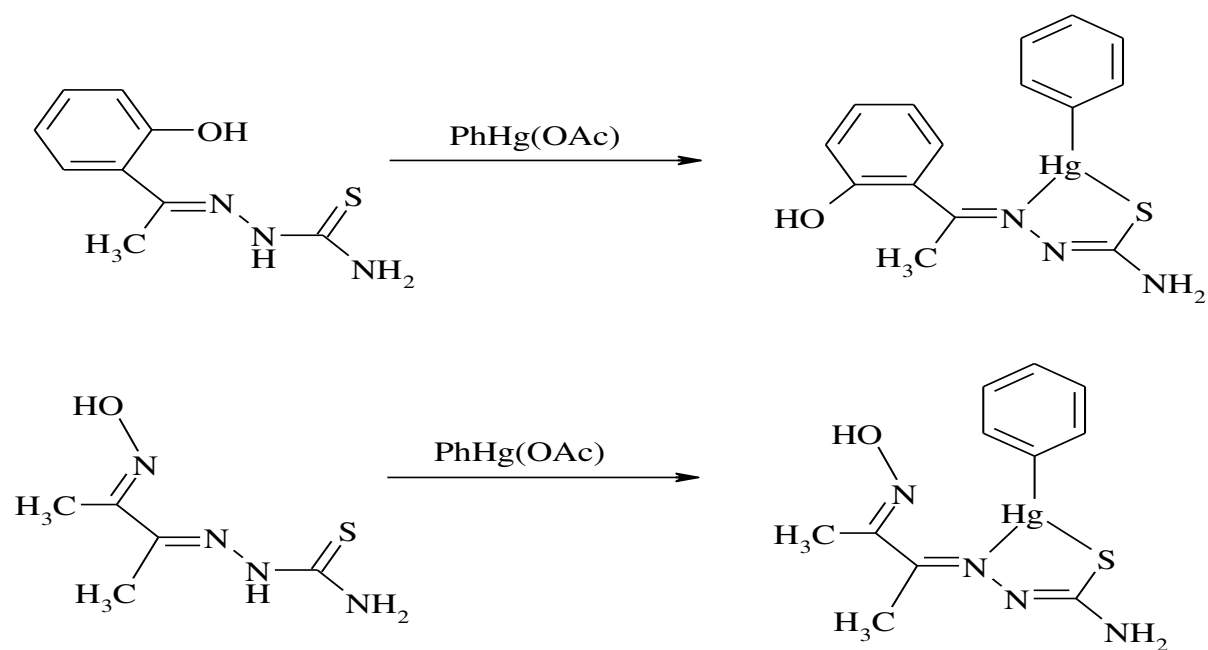
**Figure-2:** Equilibrium between the thione and thiol form of the ligands



**Figure-3:** Representative IR spectra of Haptsc



**Figure-4:** Representative electronic spectra of Hdmtsc



**Scheme-1:** Formation of Phenylmercury Schiff base complexes