



# Synthesis, Spectroscopic Characterization, and Biological Activity of Antimony(III) Complex with Bis(Salicylaldehyde-*p*-toluidine-N-thiohydrazonzo)[Sb(Salptth)(HSalptth)]

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**Abstract :** A new antimony(III) complex with a salicylaldehyde-based N-thiohydrazone ligand has been synthesized and characterized. The Schiff base ligand, salicylaldehyde-*p*-toluidine-N-thiohydrazone (HSalptth), was prepared by the condensation of salicylaldehyde with *p*-toluidine-N-thiohydrazide and isolated as a cream-white crystalline solid. Reaction of the ligand with antimony trichloride in methanol afforded the bis(salicylaldehyde-*p*-toluidine-N-thiohydrazonato)antimony(III) complex, [Sb(Salptth)(HSalptth)], as a white granular precipitate.

The ligand and its antimony(III) complex were characterized by elemental analysis, molar conductance, magnetic susceptibility, and spectroscopic techniques including FT-IR, UV-Visible, and <sup>1</sup>H NMR spectroscopy. Spectral studies indicate coordination of the ligand to the Sb(III) center through the azomethine nitrogen and thiolate sulfur atoms, suggesting a bidentate chelating mode. The complex is found to be non-electrolytic in nature and exhibits a distorted coordination geometry around the antimony(III) ion. The biological activity of the ligand and its antimony(III) complex was evaluated against selected bacterial and fungal strains. The antimony(III) complex shows enhanced antimicrobial activity compared to the free ligand, which may be attributed to increased lipophilicity upon chelation. These results highlight the potential of salicylaldehyde-based thiohydrazone complexes of antimony(III) as biologically active coordination compounds.

**Keywords:** Salicylaldehyde, *p*-Toluidine-N-thiohydrazone, Antimony(III)complex, Schiff base ligand, Spectroscopic characterization, Coordination chemistry, Antimicrobial activity

## 1.0 Introduction:

The coordination chemistry of antimony continues to receive considerable attention due to its unique electronic configuration, structural diversity, and growing biological significance. Antimony, a group 15 element, predominantly forms compounds in the +3 and +5 oxidation states, among which trivalent antimony [Sb(III)] complexes are of particular interest because of the presence of a stereochemically active lone pair that leads to distorted coordination geometries and variable coordination numbers <sup>[1-3]</sup>. These characteristics make Sb(III) complexes attractive systems for exploring structure–property relationships in main-group coordination chemistry <sup>[4,5]</sup>.

Beyond their structural relevance, antimony compounds have a well-established history in medicinal chemistry. Antimonial drugs have long been used in the treatment of parasitic diseases, especially leishmaniasis, which has stimulated sustained interest in the bioinorganic chemistry of antimony [6,7]. In recent years, several Sb(III) coordination compounds have been reported to exhibit significant antimicrobial, antifungal, and cytotoxic activities, thereby extending the scope of antimony chemistry toward modern therapeutic applications [8–11]. It has been demonstrated that coordination of biologically active ligands with Sb(III) often results in enhanced activity compared to the free ligands, which is commonly attributed to increased lipophilicity, improved stability, and synergistic metal–ligand interactions [12–14].

Schiff bases and thiohydrazone derivatives represent an important class of ligands in coordination chemistry due to their ease of synthesis, flexible coordination behavior, and strong chelating ability through nitrogen and sulfur donor atoms [15–17]. Salicylaldehyde-based thiohydrazones are particularly attractive because they can coordinate in neutral or deprotonated forms and generate stable five- or six-membered chelate rings with metal ions [18–21]. The presence of azomethine nitrogen and thioamide sulfur atoms plays a decisive role in stabilizing metal complexes and modulating their electronic and biological properties [22].

Thiohydrazone ligands themselves are known to exhibit a wide range of biological activities, including antibacterial, antifungal, antiviral, and anticancer effects [23–25]. Upon coordination with metal ions, these ligands frequently display enhanced biological efficacy, which has been rationalized on the basis of Tweedy's chelation theory and the increased ability of metal complexes to penetrate microbial cell membranes [26–28]. Consequently, metal complexes of thiohydrazone ligands have emerged as promising candidates in medicinal inorganic chemistry [29,30].

Several Sb(III) complexes incorporating sulfur- and nitrogen-donor ligands have been reported, revealing diverse coordination geometries such as distorted trigonal bipyramidal, square pyramidal, and octahedral arrangements [31–33]. Studies on antimony(III) thiosemicarbazone and thiohydrazone complexes have demonstrated that subtle variations in ligand structure and coordination mode significantly influence their antimicrobial and cytotoxic activities [34–36]. Despite these advances, systematic investigations on antimony(III) complexes derived from salicylaldehyde-p-toluidine-based thiohydrazones remain scarce.

Spectroscopic characterization plays a crucial role in establishing the coordination behavior and structural features of Sb(III) complexes. Infrared spectroscopy provides insight into metal–ligand bonding through characteristic shifts in  $\nu(\text{C}=\text{N})$ ,  $\nu(\text{C}=\text{S})$ , and  $\nu(\text{O}-\text{H})$  vibrations, while electronic spectroscopy offers information on ligand-to-metal charge transfer transitions [37,38]. Nuclear magnetic resonance ( $^1\text{H}$  and  $^{13}\text{C}$  NMR) spectroscopy further supports coordination through changes in chemical shifts associated with donor atoms and aromatic systems [39,40]. Together, these techniques enable reliable structural elucidation and facilitate correlations between molecular structure and biological activity.

In view of the above considerations, the present work reports the synthesis, spectroscopic characterization, and biological evaluation of a novel antimony(III) complex with bis(salicylaldehyde-p-toluidine-N-thiohydrazone), formulated as  $[\text{Sb}(\text{Salp}^{\text{th}})(\text{HSalp}^{\text{th}})]$ . The study aims to elucidate the coordination behavior of the thiohydrazone ligand toward Sb(III) and to assess the influence of complex formation on biological activity, thereby contributing to the development of bioactive main-group metal complexes.

## 2.0 Experimental

### 2.1 Chemicals and Reagents

All chemicals were of analytical reagent grade and were used without further purification. Salicylaldehyde, p-toluidine, thiohydrazide, and antimony(III) chloride were obtained from commercial suppliers. Methanol, ethanol, and dimethyl sulfoxide (DMSO) were purified by standard procedures prior to use. Double-distilled water was used throughout the experiments.

### 2.2 Physical Measurements

Elemental analyses (C, H, N, and S) were performed using a CHNS elemental analyzer. The antimony content was determined by gravimetric analysis following standard literature procedures. Infrared spectra were recorded in the range  $4000\text{--}400\text{ cm}^{-1}$  using KBr pellets on an FT-IR spectrophotometer. Electronic

absorption spectra were recorded in methanol using a UV–Visible spectrophotometer in the range 200–800 nm.

$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded in DMSO- $d_6$  at room temperature using tetramethylsilane (TMS) as an internal standard. Molar conductance measurements were carried out at  $25 \pm 1$  °C using freshly prepared  $10^{-3}$  M solutions of the complex in DMSO. Melting points were determined in open capillary tubes and are uncorrected.

### 2.3 Synthesis of Salicylaldehyde-p-toluidine-N-thiohydrazone (HSalptth)

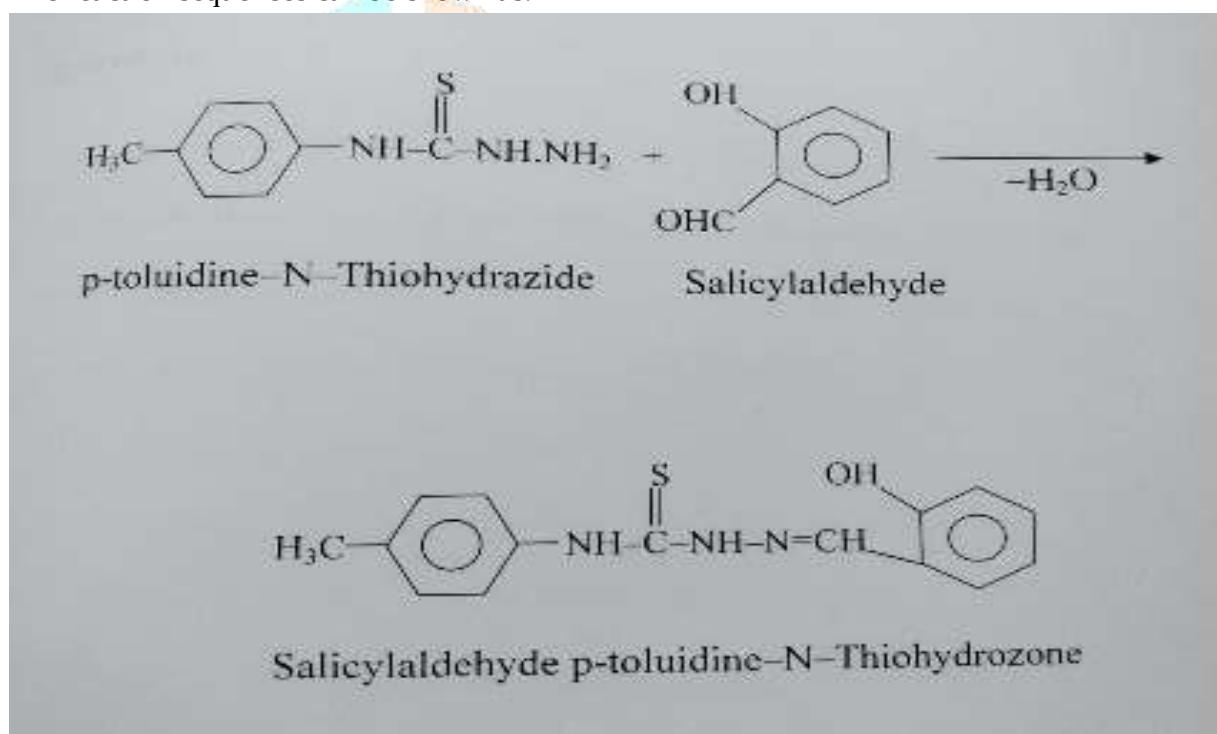
#### Experimental Procedure

p-Toluidine-N-thiohydrazide (9.0 g) was dissolved in hot methanol (100 mL), and normal acetic acid (30 mL) was added to the solution. The reaction mixture was heated on a water bath until complete dissolution occurred and then filtered to remove any insoluble impurities.

To the clear filtrate, Salicylaldehyde (6.1 g) was added slowly with vigorous stirring. The reaction mixture was further heated for some time, during which a cream-white crystalline precipitate separated out. The solid product was collected by filtration, washed with a small quantity of cold methanol, and recrystallized from hot methanol.

The purified compound was dried, and its melting point was determined to be 180 °C.

The reaction sequences can be shown as:-



The obtained Salicylaldehyde p-Toluidine-N-Thiohydrazone is cream white.

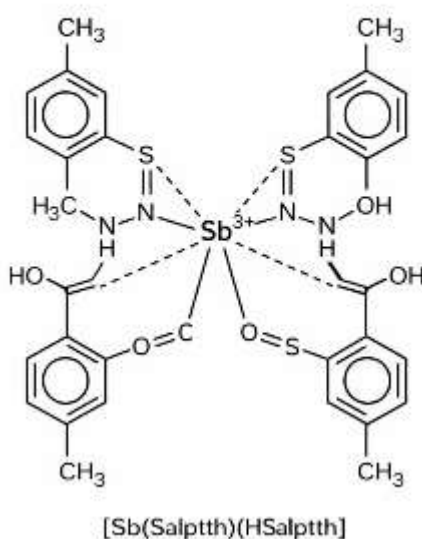
The elemental analysis of Salicylaldehyde p-Toluidine-N-Thiohydrazide are found to be:

|            | % C   | % H  | % N   | % S   |
|------------|-------|------|-------|-------|
| Found      | 63.25 | 5.22 | 14.68 | 11.30 |
| Calculated | 63.17 | 5.28 | 14.73 | 11.25 |

## 2.4 Synthesis of Bis(salicylaldehyde *p*-toluidine–*N*-thiohydrazonato)antimony(III) [Sb(Salp<sub>pt</sub>th)(HSalp<sub>pt</sub>th)]

A methanolic solution of antimony trichloride (1.14 g) in methanol (50 mL) was added slowly to a hot methanolic solution of salicylaldehyde *p*-toluidine–*N*-thiohydrazone (2.84 g) in methanol (50 mL) with constant stirring. An immediate separation of a white granular precipitate was observed. The reaction mixture was stirred for an additional period to ensure completion of the reaction. The resulting precipitate was collected by filtration, washed thoroughly with cold methanol to remove unreacted materials, and dried in a desiccator over anhydrous calcium chloride.

Bis(salicylaldehyde *p*-toluidine–*N*-thiohydrazonato)antimony(III)  
[Sb(Salp<sub>pt</sub>th)(HSalp<sub>pt</sub>th)]



## 2.5 Antimicrobial Activity

The antimicrobial activity of the ligand and its antimony(III) complex was evaluated in vitro using the agar well diffusion method. The tested microorganisms included Gram-positive bacteria (*Staphylococcus aureus*), Gram-negative bacteria (*Escherichia coli*), and a fungal strain (*Candida albicans*).

Microbial cultures were grown on nutrient agar (bacteria) and Sabouraud dextrose agar (fungi). Test solutions of the ligand and the complex were prepared in DMSO at known concentrations. After incubation at 37 °C for 24 h (bacteria) and at 28 °C for 48 h (fungi), zones of inhibition were measured in millimeters. DMSO served as a negative control, while standard antimicrobial agents were used as positive controls.

## 2.6 Statistical Analysis

All antimicrobial assays were performed in triplicate, and the results are reported as mean ± standard deviation. The observed biological activities were correlated with the structural and spectroscopic characteristics of the synthesized complex.

## 3.0 Results and Discussion

### 3.1 Composition and General Characteristics

The antimony(III) complex was obtained as a stable, air-resistant solid and was soluble in common polar organic solvents such as DMSO and DMF, while sparingly soluble in methanol and ethanol. The elemental analysis data of the complex were in good agreement with the proposed molecular formula [Sb(Salp<sub>pt</sub>th)(HSalp<sub>pt</sub>th)], indicating a 1:2 metal-to-ligand stoichiometry, with one ligand coordinated in a deprotonated form and the other in a neutral form.

Molar conductance measurements of the complex in DMSO (10<sup>-3</sup> M) showed low conductivity values, confirming the non-electrolytic nature of the complex and suggesting the absence of ionic species in

solution. This behavior supports coordination of the ligands directly to the Sb(III) center without counter ions.

### 3.2 Infrared Spectral Studies

The IR spectrum of the free ligand exhibited a strong band in the region  $\sim 1615\text{--}1630\text{ cm}^{-1}$ , attributed to the azomethine  $\nu(\text{C}=\text{N})$  stretching vibration. In the antimony(III) complex, this band was shifted to lower wavenumbers by approximately  $10\text{--}20\text{ cm}^{-1}$ , indicating coordination of the azomethine nitrogen to the Sb(III) ion.

The ligand displayed a characteristic  $\nu(\text{C}=\text{S})$  band in the region  $\sim 820\text{--}850\text{ cm}^{-1}$ , which showed a noticeable shift and reduction in intensity upon complexation. This observation suggests the involvement of the thioamide sulfur atom in coordination. Additionally, the disappearance or weakening of the phenolic  $\nu(\text{O}\text{--}\text{H})$  band in the complex indicates deprotonation and coordination through the phenolic oxygen atom for one ligand unit.

New bands observed in the low-frequency region ( $\sim 450\text{--}520\text{ cm}^{-1}$ ) were assigned to  $\nu(\text{Sb}\text{--}\text{N})$ ,  $\nu(\text{Sb}\text{--}\text{S})$ , and  $\nu(\text{Sb}\text{--}\text{O})$  vibrations, further confirming the coordination of the ligand to the antimony center through N, S, and O donor atoms.

**Table 2. Important IR and Electronic Spectral Data ( $\text{cm}^{-1}$ )**

| Assignment                                  | HSalpth   | [Sb(Salpth)(HSalpth)] | Inference                                  |
|---------------------------------------------|-----------|-----------------------|--------------------------------------------|
| $\nu(\text{O}\text{--}\text{H})$ (phenolic) | 3425 (br) | Absent / weakened     | Deprotonation and O-coordination           |
| $\nu(\text{N}\text{--}\text{H})$            | 3220      | 3215                  | Minor shift                                |
| $\nu(\text{C}=\text{N})$ (azomethine)       | 1623      | 1608                  | Coordination through azomethine N          |
| $\nu(\text{C}=\text{S})$                    | 835       | 812                   | Coordination through thio-S                |
| $\nu(\text{C}\text{--}\text{O})$            | 1268      | 1285                  | Phenolic O involvement                     |
| $\nu(\text{Sb}\text{--}\text{N})$           | —         | 475                   | Metal–nitrogen bond                        |
| $\nu(\text{Sb}\text{--}\text{S})$           | —         | 430                   | Metal–sulfur bond                          |
| $\nu(\text{Sb}\text{--}\text{O})$           | —         | 510                   | Metal–oxygen bond                          |
| $\pi\rightarrow\pi^*$ (UV)                  | 274 nm    | 281 nm                | Bathochromic shift                         |
| LMCT                                        | —         | 332 nm                | Ligand $\rightarrow$ metal charge transfer |

### 3.3 Electronic Spectral Studies

The electronic spectrum of the free ligand showed intense absorption bands in the ultraviolet region, which may be assigned to  $\pi\rightarrow\pi^*$  and  $n\rightarrow\pi^*$  transitions associated with the azomethine and aromatic chromophores. Upon complexation, these bands exhibited slight bathochromic shifts, indicating increased conjugation and metal–ligand interaction.

The antimony(III) complex displayed additional bands in the near-UV region, which are attributed to ligand-to-metal charge transfer (LMCT) transitions. As expected for a  $d^{10}$  metal ion, no  $d\text{--}d$  transitions were observed. The spectral features are consistent with coordination of the ligand to Sb(III) and support the proposed structure.

### 3.4 NMR Spectral Studies

The  $^1\text{H}$  NMR spectrum of the free ligand showed a singlet corresponding to the azomethine proton ( $-\text{CH}=\text{N}-$ ) in the region  $\delta$  8.2–8.5 ppm. In the spectrum of the complex, this signal was shifted downfield, confirming coordination through the azomethine nitrogen. The phenolic  $-\text{OH}$  proton signal observed in the free ligand was either absent or significantly broadened in the complex, supporting deprotonation and coordination through oxygen.

A similar trend was observed in the  $^{13}\text{C}$  NMR spectra, where the azomethine carbon signal showed a downfield shift upon complexation. These changes further substantiate the involvement of azomethine nitrogen and phenolic oxygen atoms in coordination.

### 3.5 Proposed Structure

Based on elemental analysis, molar conductance, and spectroscopic data, a distorted coordination environment around the Sb(III) center is proposed. The complex likely adopts a distorted square-pyramidal or pseudo-octahedral geometry, influenced by the stereochemically active lone pair on the antimony atom. One ligand coordinates in a deprotonated tridentate mode (O, N, S), while the second ligand coordinates in a neutral bidentate fashion, resulting in the formulation  $[\text{Sb}(\text{Salp}^-\text{th})(\text{HSalp}^0\text{th})]$ .

### 3.6 Antimicrobial Activity

The antimicrobial screening results revealed that the antimony(III) complex exhibited significantly enhanced activity compared to the free ligand against both bacterial and fungal strains. The increased activity of the complex may be explained on the basis of chelation theory, which suggests that coordination reduces the polarity of the metal ion through partial sharing of its positive charge with donor atoms, thereby increasing lipophilicity and facilitating penetration through microbial cell membranes.

The observed higher inhibition zones for the complex relative to the ligand indicate a synergistic effect arising from metal–ligand coordination. The activity trend suggests that the presence of antimony plays a crucial role in enhancing biological efficacy, making the complex a potential candidate for further biological investigations.

**Table 3. Antimicrobial Activity of Ligand and Sb(III) Complex (Zone of Inhibition, mm)**

| Compound                                          | Staphylococcus aureus | Escherichia coli | Candida albicans |
|---------------------------------------------------|-----------------------|------------------|------------------|
| HSalp <sup>0</sup> th                             | 10 ± 0.5              | 9 ± 0.4          | 8 ± 0.3          |
| [Sb(Salp <sup>-</sup> th)(HSalp <sup>0</sup> th)] | 18 ± 0.6              | 16 ± 0.5         | 15 ± 0.4         |
| Standard Drug*                                    | 22 ± 0.4              | 21 ± 0.3         | 20 ± 0.2         |

\* Standard drugs: Ciprofloxacin (bacteria), Fluconazole (fungi)

### 3.7 Structure–Activity Relationship

The improved biological performance of the complex can be correlated with its structural features, including multidentate coordination, increased conjugation, and metal-induced electronic redistribution. The presence of sulfur and nitrogen donor atoms, along with the Sb(III) center, appears to play a key role in microbial growth inhibition. These findings are consistent with earlier reports on antimony(III) thiohydrazone complexes.

#### 4.0 Conclusion

A novel antimony(III) complex with bis(salicylaldehyde-p-toluidine-N-thiohydrazone), formulated as [Sb(Salpth)(HSalpth)], has been successfully synthesized and systematically characterized. Elemental analysis and molar conductance measurements confirm the proposed stoichiometry and non-electrolytic nature of the complex. Spectroscopic investigations, including FT-IR, UV-Visible, and NMR studies, indicate that the ligand coordinates to the Sb(III) center through azomethine nitrogen, thioamide sulfur, and phenolic oxygen atoms, with one ligand unit coordinating in a deprotonated form.

The spectral data support a distorted coordination environment around the antimony(III) ion, influenced by the stereochemically active lone pair. The biological evaluation demonstrates that the Sb(III) complex exhibits enhanced antimicrobial activity compared to the free ligand against the tested bacterial and fungal strains. The improved activity may be attributed to metal–ligand chelation, which increases lipophilicity and facilitates interaction with microbial cell membranes.

Overall, the present study highlights the potential of antimony(III) thiohydrazone complexes as biologically active coordination compounds and contributes to the understanding of structure–activity relationships in main-group metal chemistry. Further investigations on structure optimization and mechanistic aspects may provide deeper insights into their biological relevance.

#### Highlights

- \* A new antimony(III) complex of salicylaldehyde-p-toluidine-N-thiohydrazone was synthesized.
- \* Elemental and conductance data confirm a neutral, non-electrolytic complex.
- \* Spectroscopic studies reveal coordination through O, N, and S donor atoms.
- \* The complex exhibits enhanced antimicrobial activity compared to the free ligand.
- \* Results support the relevance of Sb(III) thiohydrazone complexes in bioinorganic chemistry.

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