

# Comprehensive Investigation of Thermal and Biological Properties of novel boron based Metal Complex

<sup>1</sup>Arun Tomar, <sup>2</sup> Dr Rajeev Rathore

<sup>1</sup>Research Scholar, <sup>2</sup> Associate professor

Department of Chemistry

Meerut college, Western Kutchery Rd, Lalkurti Bazaar, Begambagh, Meerut, Uttar Pradesh, India 250003

Kumar.arun.arun041@gmail.com

**Abstract :** This research presents a comprehensive exploration of the thermal and biological properties of newly synthesized Boron(II) complexes derived from 2-[di(2,3-dihydro-1H-indol-3-yl)]ligands. The synthesis of these compounds involved the utilization of various 2-[di(2,3-dihydro-1H-indol-3-yl)]ligands, followed by rigorous characterization using multiple analytical techniques, including <sup>1</sup>H NMR, IR, <sup>13</sup>C NMR, elemental analysis, and UV spectroscopy for the ligands. Furthermore, the resulting complexes were extensively characterized through elemental analysis, UV spectroscopy, IR spectroscopy, and thermal analysis techniques, including TGA/DTG and DSC. In addition, biological potential of these compounds was evaluated through antibacterial testing. The findings unveiled promising antibacterial properties, underscoring their potential for further exploration in the realm of antimicrobial agents.

**Introduction:** For nearly a century, heterocycles have become the focus of some of the most in-depth research in organic chemistry. It has had a significant impact on the biological and industrial development of civilization, as well as the investigation of biological processes and initiatives that improve quality of life [1] Boron-containing compounds have garnered significant attention across diverse scientific disciplines due to their unique chemical properties and wide-ranging applications, from materials science to medicinal chemistry.[2] Within this family of compounds, boron based 2-[di(2,3-dihydro-1H-indol-3-yl)]ligands represent a class of molecules with potential utility in catalysis, sensing, and biological applications.[3] While these ligands' synthesis and structural characterization have been explored,[4] a comprehensive understanding of their thermal behavior and biological activities remains limited. This study addresses this gap by investigating the thermal properties and biological activities of a series of novel boron 2-[di(2,3-dihydro-1H-indol-3-yl)] ligands. This research aims to provide valuable insights into the structure-property relationships of these compounds and their potential applications in various fields.

The study of boron based 2-[di(2,3-dihydro-1H-indol-3-yl)]ligands has garnered significant attention in recent years due to their unique thermal and biological properties, making them highly suitable for catalysis, material science, and medicinal chemistry applications. [5] The incorporation of boron into organic frameworks offers an opportunity to enhance chemical stability and reactivity, while the 2-[di(2,3-dihydro-1H-indol-3-yl)]ligands moiety is well-known for its versatile coordination behavior and biological activities, such as antimicrobial and anti-inflammatory effects.

Exploration of the thermal properties of these ligands is essential for understanding their stability and potential as components in high-temperature applications, such as advanced materials and thermal storage systems [6]. Simultaneously, their biological properties hold promise for developing new pharmaceuticals and bioactive compounds. The intersection of these fields underscores the importance of a comprehensive investigation into the structural, thermal, and biological characteristics of boron based 2-[di(2,3-dihydro-1H-indol-3-yl)]ligands.

Schiff bases, first reported by Hugo Schiff in 1864, are condensation products of primary amines with carbonyl compounds, typically aldehydes or ketones. These compounds are characterized by the azomethine (-CH=N-) functional group, which imparts unique chemical and biological properties [8]. The versatility of Schiff bases lies in their structural diversity, which can be fine-tuned by altering the amine or carbonyl precursors. This flexibility makes Schiff bases valuable in various fields, including coordination chemistry, catalysis, material science, and medicinal chemistry [9,10].

The formation of Schiff bases is often a simple and efficient process, with the reaction typically proceeding under mild conditions and yielding high purity products. This reaction mechanism involves nucleophilic addition of the amine to the carbonyl group, followed by dehydration to form the azomethine linkage. The ease of synthesis, combined with their ability to act as ligands, allows Schiff bases to coordinate with metal ions, forming stable and often biologically active metal complexes [11].

In addition to their chemical versatility, Schiff bases exhibit a wide range of biological activities, including antimicrobial, antifungal, and anticancer properties. Their pharmacological potential arises from their ability to interact with various biological targets, often through the azomethine group [12]. Consequently, Schiff base chemistry has become an active area of research aimed at designing novel compounds with enhanced biological activity.

### Material and Analytical support:

All material purchased from local market and and Metal source purchase from Sigma Aldrich.TLC plate from merck,and analytical support from NFDD-Rajkot and Sathi-Banaras Hindu University.

**Methods:** FT-IR spectra were recorded as KBr pallets on Thermo fisher Nicolet-400D spectrophotometer from NFDD-Rajkot.1H NMR spectra were recorded on Advance 600 Bruker FT-NMR instrument in DMSO-d6 solvent from SATHI-Bnanaras Hindu University. The FAB-mass spectrum of heterochelate was analyzed by JEOL SX-102/DA-6000 mass spectrometer from local testing lab. Simultaneous TGA/DTG and DSC were obtained by a model 5000/2960 SDT. The experiment was performed in under inert Condition of N2 gas at heating rate of 10°Cmin<sup>-1</sup>.

### General Procedure:

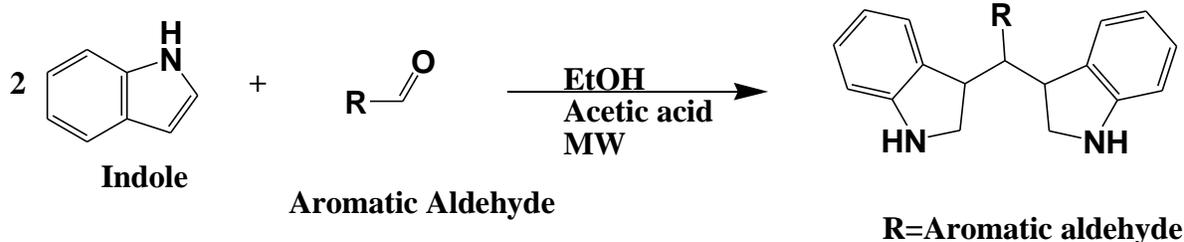
#### MATERIALS AND METHODS:

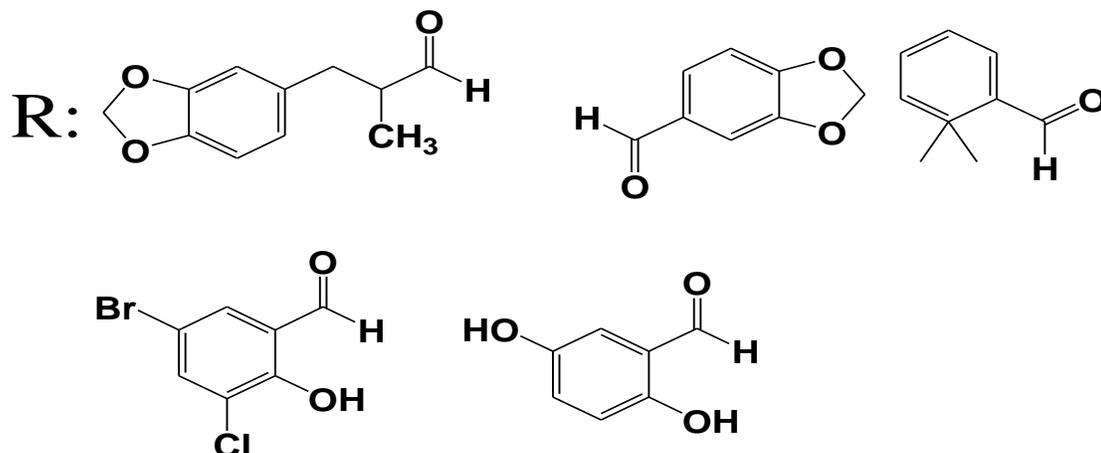
This section discusses the reagents used, as well as the various analytical and physicochemical techniques used in the characterization experiments. It also includes the production and analysis of ligands and transition metal complexes used in the latest research.

### Synthesis of Schiff Base Ligands:

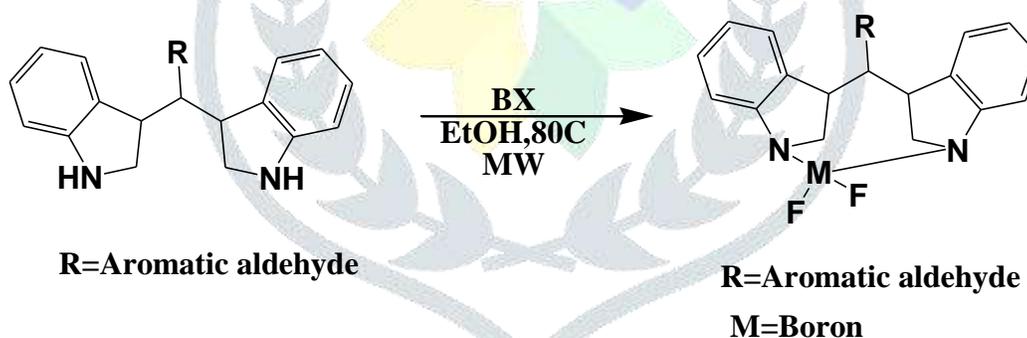
#### Step-01

Take a 50 mL round-bottom flask (RBF) fitted with a reflux condenser and set the system for reflux with gentle stirring. Charge **0.50 mmol of indole** and **0.25 mmol of aromatic aldehyde**,add **5-7 volumes of ethanol** as the solvent, add catalytic amount (a few drops) of **acetic acid** to the reaction mixture, and reflux the mixture at **78°C** (boiling point of ethanol) for **6 hours**. Monitor the progress of the reaction using thin-layer chromatography (TLC) at regular intervals. Recrystallize the crude product using ethanol to purify the Schiff base ligand. Complexation with Boron.



**Mw: Microwave irradiation****Step-02**

Dissolve the purified Schiff base ligand in a suitable solvent such as **toluene** or **methanol** (10–20 mL, depending on the scale). add a boron source (e.g., boron trihalide [BCl<sub>3</sub>], phenylboronic acid, or BF<sub>3</sub>) dropwise to the solution. Maintain constant stirring during the addition to avoid localized overheating or decomposition. [Boron typically coordinates with the nitrogen atom of the azomethine (-CH=N-) group, and it may also interact with hydroxyl groups if present (e.g., in salicylaldehyde-based Schiff bases). Reflux the mixture at 80°C for 4–6 hours under an inert atmosphere (e.g., nitrogen gas) to promote complete complexation. Monitor the reaction for completion, often indicated by a distinct color change in the solution. Allow the reaction mixture to cool to room temperature. If the complex precipitates, filter it using vacuum filtration and wash with cold solvent (e.g., methanol or diethyl ether), Dry the complex.

**Step-02** Boron metal binding with synthesized sulphonated ligands*Results and Discussion: NMR data & spectra of ligand*

<sup>1</sup>H NMR data of ligand for L1-L6:

**L1:** <sup>1</sup>H NMR: δ 0.73-0.85 (3H), 1.61 (1H), 2.31 (2H), 2.91 (1H), 3.38-3.68 (6H), 5.93 (2H), 6.50-6.76 (5H), 6.79-7.02 (6H)

**L3:** <sup>1</sup>H NMR: δ 1.12-1.22 (6H), 1.87 (2H), 2.12 (2H), 3.21 (1H), 3.41 (4H), 3.60 (2H), 5.56 (1H), 5.96 (1H), 6.49-6.74 (3H), 6.79-7.02 (6H).

**L4:** <sup>1</sup>H NMR: δ 3.24 (1H), 3.49 (4H), 3.66 (2H), 5.93 (2H), 6.56 (2H), 6.67-7.02 (9H).

The resonance of 2-[di(2,3-dihydro-1H-indol-3-yl)] has been extensively studied [20-24]. In DMSO-d<sub>6</sub> at room temperature, <sup>1</sup>H NMR measurements were conducted to analyse the Schiff base ligand. Details of the ligand's <sup>1</sup>H NMR spectrum are provided in the experimental section. This spectrum showed two sharp singlets in the range of 12 to 13 ppm, which correspond to one and two protons and are indicative of the -OH group. When a D<sub>2</sub>O exchange experiment was performed, this signal disappeared. While singlets for the

methyl group in the Schiff base ligands emerged in the range of 1.5 to 3.0 ppm, aromatic protons were seen in the range of 6.8 to 9.0 ppm. It was difficult to clearly identify each signal as belonging to a particular aromatic or -NH proton because it was revealed by the NMR spectrum of L1 that the signals of -NH protons occasionally overlapped with those of aromatic protons. It was determined from the  $^1\text{H}$  NMR spectroscopic data that the Schiff base ligand occurs in solution as the keto-enol form.

FT-IR Data of ligand:

Ligands	$\nu$ (O-H)	$\nu$ (N-H)	$\nu$ (C=O)	$\nu$ (C=N)
L1	3342	3256	1612	1568
L2	3240	3289	1607	1554
L3	3352	3301	1610	1534
L4	3348	3198	1598	1525
L5	3349	3296	1629	1519
L6	3241	3245	1619	1529

Figure 1:  $^1\text{H}$  NMR Spectra of ligand [L1]

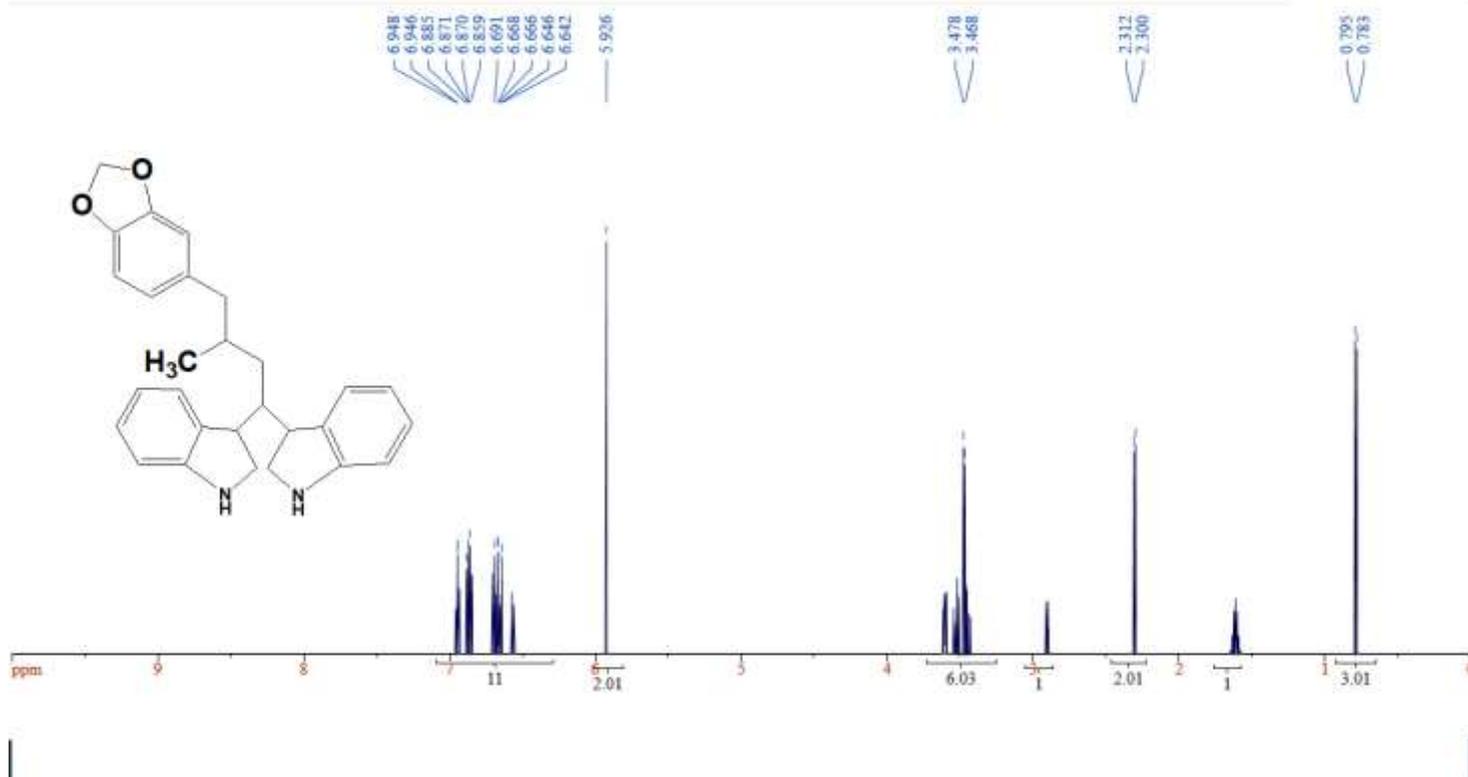


Figure 2: <sup>13</sup>C NMR Spectra of ligand [L1]

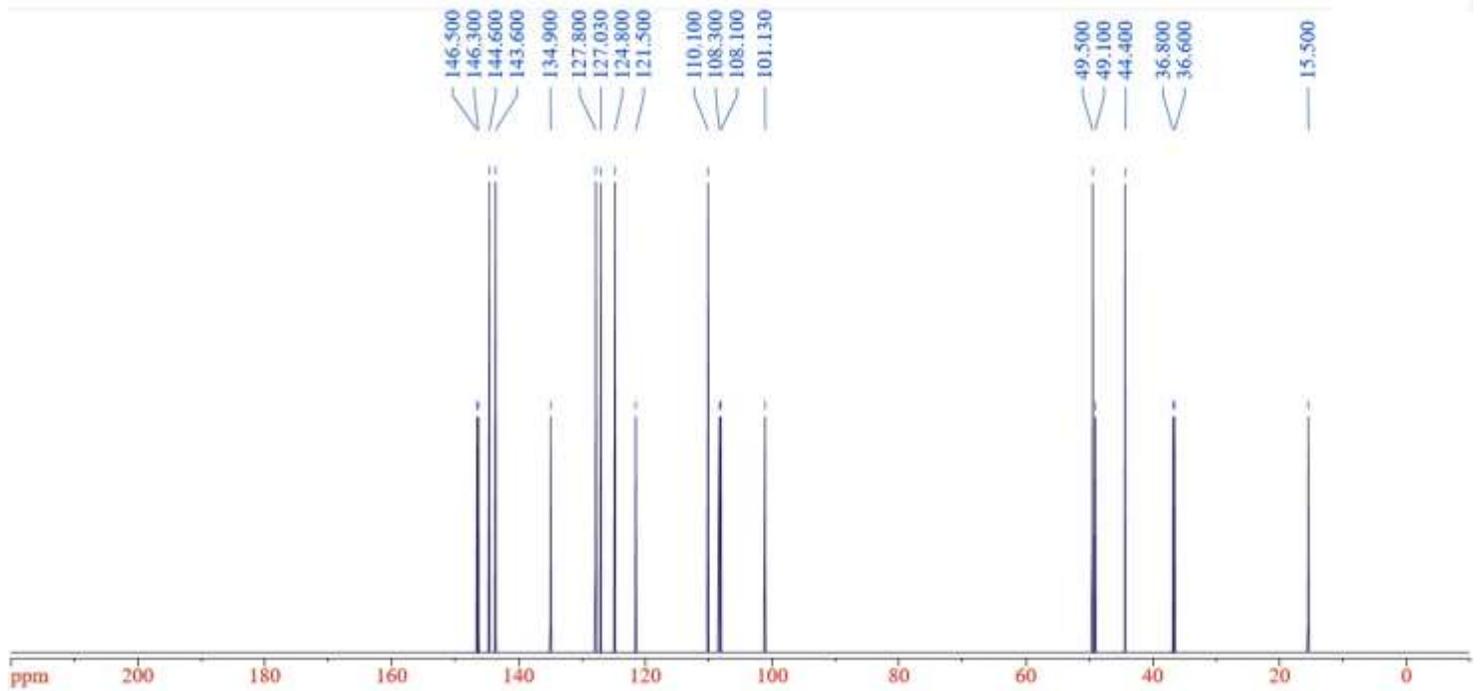
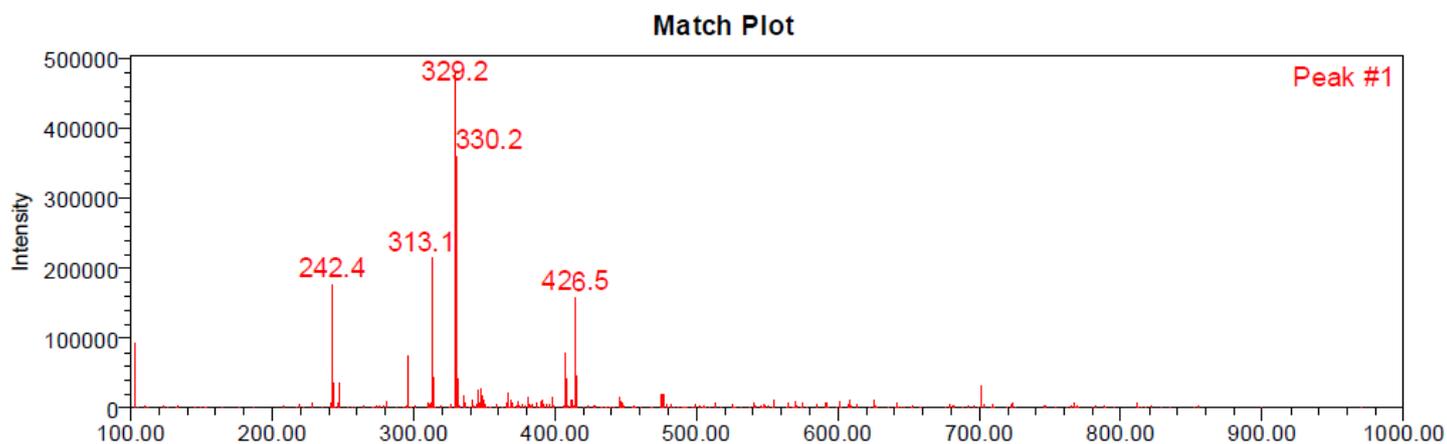


Figure 4: Mass Spectra of ligand [L1]



### Conclusion

The design and synthesis of new Schiff base ligand have been successfully demonstrated FT-IR and <sup>1</sup>H NMR and Mass Spectral studies reveal that ligand exists in tautomeric enol form both in solid and solution state with intra molecular N-H-bonding. We have synthesized a series of some novel Boron (III) heterochelates with boron 2-[di(2,3-dihydro-1*H*-indol-3-yl)] ligands derivative and characterize their properties. All the synthesized compounds were screened for their bioassay. The heterochelates exhibit strong activities against Gram+ve (*Bacillus Magaterium*) and Gram-ve (*E.coli*) organisms in comparison with ligand and drug penicillin. Some of the ligands and heterochelates were more active against one or more bacterial strain introducing a novel class of metal based bactericidal agents.

Table3: Antimicrobial Effects of the Ligands and their Heterochelates

Sr. No.	Compounds	Gram <sup>+ve</sup>	Gram <sup>-ve</sup>
		<i>Bacillus Megaterium</i>	<i>E.Coli</i>
Ref. Drug	Penicillin	45	30
1	L <sub>1</sub>	20	16
2	L <sub>2</sub>	17	12
3	L <sub>3</sub>	10	14
4	L <sub>4</sub>	<b>30</b>	<b>55</b>
5	L <sub>5</sub>	10	<b>25</b>
6	AL <sub>1</sub>	11	09
7	AL <sub>2</sub>	25	<b>20</b>
8	AL <sub>3</sub>	<b>33</b>	<b>15</b>
9	AL <sub>4</sub>	23	11
10	AL <sub>5</sub>	23	08

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