

## Design, Synthesis, And Solid-State Emissive Properties of Sulphanilamide-Derived Schiff Bases: Biological Evaluation and Thin Film Applications

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### ABSTRACT:

The goal of the multidisciplinary area of crystal engineering is to precisely manage intermolecular interactions such as hydrogen bonding,  $\pi$ - $\pi$  stacking, and van der Waals forces in order to create and build crystalline materials with specific features. Utilizing techniques like co-crystallization, polymorphism, and molecular templating to maximize structural and functional features, it is used in fields including medicines, optoelectronics, and catalysis. Solid-state organic emitters are materials that, because of their  $\pi$ -conjugated architectures, exhibit fluorescence, phosphorescence, or thermally activated delayed fluorescence (TADF). These materials are essential for technologies such as OLEDs, lasers, and sensors. For optimal performance, advanced design techniques minimize aggregation-caused quenching (ACQ) and increase aggregation-induced emission (AIE). By combining crystal engineering with organic emitters, issues like stability, scalability, and environmental impact may be addressed and emission properties can be fine-tuned using co-crystals, polymorphism, and host-guest systems. Organic luminescent Schiff bases require the understanding of their molecular structure, intermolecular interactions, and solid-state packing arrangements to improve their luminescent properties. Thus, rational design forms the starting point for crystal engineering of organic luminescent Schiff bases. Chemists shape the molecular structure with the appropriate building blocks, for example, aromatic aldehydes and amines, as well as functional group modification to control electronic and steric properties of molecules. Thus, crystal engineering aims to optimize intermolecular interactions within the solid-state lattice for enhanced energy transfer and less-decay pathways. Hydrogen bond,  $\pi$ - $\pi$  stacking, and Vander Waal's interactions are critical in terms of orienting molecules within this framework and the resulting packing efficiency. Crystal engineering of organic luminescent Schiff bases for thin film studies and mechanofluorochromism: Molecular structures as well as the solid-state packing arrangements are made suitable to enhance the luminescence properties and material sensitivity towards mechanical stimuli. In the principles of crystal engineering, molecular packing and orientation within thin films are so optimized that both efficiency of emission and stability of film are maximized. Controlling the thickness and morphology of thin films by adjusting deposition parameters would open up investigation in the structure-property relationship and possibly test thin-film performance in optoelectronic devices. Organic luminescent Schiff bases have been designed with specific intermolecular interactions and designed solid-state packing arrangements based on the strategies of crystal engineering to provide mechanofluorochromism behavior. The disruptive change in non-covalent interactions, such as  $\pi$ - $\pi$  stacking or hydrogen bonding, under mechanical stress

affects the electronic structure and emission properties of the material. These approaches rely on the basic principles of solid-state chemistry for the adjustment of optical properties toward a range of applications in optoelectronics and sensing.

## INTRODUCTION:

### Chapter-1: CRYSTAL ENGINEERING:

#### 1.1: Overview of Crystal Engineering

Starting point in crystal engineering is often given by a definition: creation of materials with specific useful properties through molecular and crystal engineering<sup>1</sup>. The area is applied rather widely, from pharmaceuticals - enhancement of solubility and stability of drugs - to material sciences - development of new materials for electronics and sensors<sup>2</sup>. The concept is basically the ability to design and assemble molecules in a crystal lattice through knowledge of and application of intermolecular forces, such as hydrogen bonding,  $\pi$ - $\pi$  stacking, and Van der Waals forces.<sup>3-4</sup>

The term crystal engineering was first coined by Pepinsky in 1955, but modern application—and often its definition—of it as a deliberate process of creating well-defined and controlled crystalline structures is often attributed to Gerhard Schmidt<sup>5</sup>. In fact, the highly influential and pioneering work of Schmidt was especially in the area of photodimerization reactions in crystalline cinnamic acid that led to the comprehension that intermolecular arrangements really determine the properties of crystalline materials<sup>6</sup>. In that respect, the knowledge of such structural arrangements to have effects on the properties of crystals revealed how it would become possible to design crystals with predetermined properties—an insight that has gone to form the core of crystal engineering.<sup>7</sup>

A good part of crystal engineering is done through weak, non-covalent interactions responsible for the assembly and stability of its crystal structures<sup>8</sup>. These interactions include hydrogen bonds, halogen bonds, cation- $\pi$  interactions,  $\pi$ - $\pi$  interactions, and Van der Waals forces. This type of interaction, depending on the functional groups and the geometrical properties of the molecular components, uniquely contributes to crystallization<sup>9</sup>. Thus, scientists can control crystal packing, stability, and therefore functional properties of the resulting material by manipulating these molecular features. In other words, this systematic way of building molecular arrangement finds roots in early studies of molecular stacking, especially in the contributions of W.L. Bragg, J.M. Robertson, and Schmidt, who together aimed at determining the rules governing molecular stacking and packing within crystalline structures.<sup>10-11</sup>

Desiraju further formalized the description of this field as being "the understanding of intermolecular interactions associated with crystal stacking and the use of such understanding in the design of new solids with desired physical and chemical properties."<sup>12-13</sup> Such definition highly emphasizes a goal-oriented approach in material design, whereby researchers work toward a particular functionality by carefully manipulating intermolecular forces in the crystal lattice. This goal-oriented approach is particularly valuable in the design of functional molecular solids—for example, in drug and electronic applications, in which the required physical or chemical property is frequently needed.<sup>14</sup>

An important concept in crystal engineering is the supramolecular synthon, a term that Desiraju has introduced. A supramolecular synthon is an architectural unit or building block that directs the assembly of molecules into a crystal. Synthons may be designed to be functionalized or made adapted for specific needs. Thus, crystals may be prepared with special reactivity properties, selective absorption of specific molecules, optical properties, or electrical properties.<sup>15</sup> This is one of the fundamental ideas that serve as a building block for functional molecular solids. Utilizing synthons will ultimately enable scientists to be able to prepare crystals for very specific purposes-based applications—from drug delivery systems to organic electronics.<sup>16</sup> Thus, an ideal crystal is not just an assembly of molecules but a well-designed structure, designed for a particular purpose based on its supramolecular arrangement.

In the last few decades, crystal engineering has undergone tremendous evolution. Currently, this scientific discipline is no longer limited to structural aspects of crystals but elaborates on a wide range of practical applications. Applications include almost everything that functions as a protein recognition system, polymer design, drug delivery systems, and so many others.<sup>17</sup> Crystal engineering thus now cuts across many fields of sciences, which include inorganic chemistry, physical chemistry, crystallography, materials science, and computational chemistry. The interdisciplinary nature of crystal engineering further posits that it has potentials for innovative application across various fields, ranging from biomedical engineering to electronic and energy storage devices.<sup>18</sup>

Robertson's seminal early work in the early days of crystallography specially linked for the first-time supramolecular structures of organic compounds with their crystal structures. Robertson's works on crystal structures of stacked aromatic hydrocarbons, for instance, anthracene and naphthalene, are good examples of the pioneering work of how the packing in crystalline patterns impacts molecular structure to affect stability, melting points, and optical properties. His fundamental realization came from these studies that the property of crystals is not determined by the molecular composition alone but also by the spatial arrangement of molecules and their interactions.

Perhaps more directly related to crystal engineering, however, is the area of supramolecular chemistry. Nobel laureate Jean-Marie Lehn defines that branch as "the chemistry of molecular assembly and intermolecular bonding." Supramolecular chemistry is the study of how supramolecules, or molecular assemblies, assemble through non-covalent interactions.<sup>19</sup> Lehn's work focused on demonstrating how these interactions could be purposefully controlled in order to yield organized structures with special functions. In crystal engineering, principles of supramolecular chemistry are used to create materials that can perform a desired or tailored function as mediated by selective binding or higher conductivity. Through the synergy of crystal engineering and supramolecular chemistry, scientists have the right tools to design materials from the molecular level upwards, then apply these innovations in areas as widely diverse as pharmaceuticals, nanotechnology, and environmental science.<sup>20</sup>

In summary, crystalline engineering is the strategic multidisciplinary design approach to materials engineering based on the insights of intermolecular interactions and molecular organization toward a predetermined set of functions in solid-state materials. From its origin in simple crystallography through supramolecular chemistry, crystal engineering has played an innovative role in advancing materials science with novel solutions to complex scientific and industrial problems.<sup>21</sup>

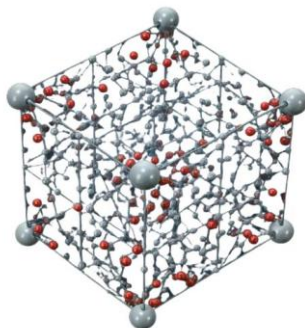


Fig 1.1: General depiction of unit cell of a reproductive crystal

### 1.2: Introduction to Schiff bases

Schiff bases are those compounds that contain a carbon-nitrogen double bond, ( $-C=N-$ ), which is derived by the condensation reaction of a primary amine with an aldehyde or a ketone. The compounds exhibit several interesting properties that make them applicable to various fields, including chemistry, biology, or materials science, among others.<sup>22</sup> More of these with details on their properties are presented below. Inorganic elements have crucial roles in biological and medical processes; it is obvious that many organic compounds used in medicine do not have a purely organic mode of action since some are activated or bio-transformed by metal ions metabolism.<sup>23</sup> Many drugs have changed toxicological as well as pharmacological properties in the form of a metal complex, and probably Schiff bases are versatile  $C=N$  (Imine) containing compounds, which possess a broad range of biological activity, and the incorporation of metals in the form of complexes showed some degree of antibacterial, antifungal, antitumor, and anti-inflammatory activity.<sup>24</sup> Schiff base is the compound containing azomethine group ( $-HC=N-$ ). They are the condensation products of ketones (or) aldehydes (aldehyde and ketones) with primary amines and were first reported by Hugo Schiff in 1864. Schiff base formation usually takes place under acids or base catalysis or with heat. The common Schiff bases are crystalline solids, which are feebly basic but at least some form insoluble salts with strong acids. Schiff base are used as an intermediate in the synthesis of amino acids or as a ligand in the Preparation of metal complexes having a series of different structures.

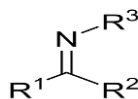
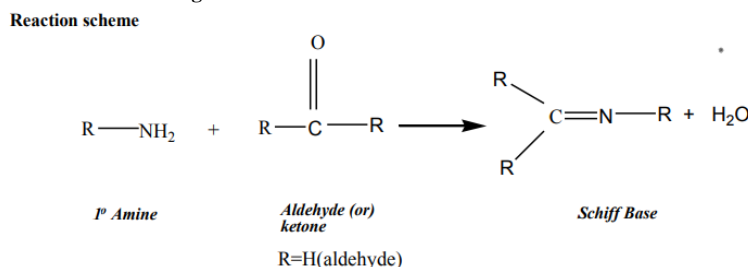


Fig. 1.2: General structure of Schiff base



### 1.3: Properties of Schiff bases

Schiff bases are organic compounds containing an imine or azomethine -C=N- linkage functional group. They are prepared by a condensation reaction in which a carbonyl compound (aldehyde or ketone) reacts with a primary amine to produce a compound known as a Schiff base. This has some interesting properties that make it highly relevant in chemistry, biochemistry, and even materials science.<sup>25</sup>

They have the ability to form complexes with transition metal ions common feature of Schiff bases. They play the role of L-type ligands in these complexes, that is, ligands, which contain donors of two electrons, who do not experience electron redistributions on their valence shells.<sup>26</sup> This coordination of the d-block metal ion by the electron-donating ligand atom results in complex formation and is intended to modify the steric and electronic surrounding of the metal. This, therefore, leads to the stabilization and regulation of the reactivity of the metal ion very highly useful in the case of less stable ions at higher oxidation states. Nitrogen, oxygen or sulphur atoms can be donors and be involved in the coordination.<sup>27</sup>

Schiff bases also possess structural diversity due to the way synthesis is carried out, such that any combinations of amines and carbonyl compounds can be synthesized. This is potentially a promising approach for realizing Schiff bases with their various properties tailored toward a specific application.

Schiff bases and their metal complexes exhibit antimicrobial, anticancer, antioxidant activities, and enzyme inhibition activity. Such a combination of properties implies great potential for Schiff bases as promising candidates for drugs in medicinal chemistry.<sup>28</sup>

This means that Schiff bases have a very wide range of properties that make these compounds rather versatile in many areas, such as coordination chemistry, materials science, biology, and medicinal chemistry. Due to structural diversity and tunability of their properties, Schiff bases are very attractive targets for much research and development work in many different areas of science and technology.

### 1.4: Introduction to Solid state emissive organic molecules

The area of intersection of material science and photo physics has been an exciting one. It led to some outstanding advances in the theory and design of solid-state emissive organic molecules.<sup>29</sup> In recent years, tremendous interest has been generated in such materials with strong luminescence in the solid state toward applications in organic light-emitting diodes (OLEDs), lasers, sensors, bioimaging, and energy conversion technologies.<sup>30</sup> Unlike typical dyes, which often face aggregation-caused quenching (ACQ) problems in the solid state, SSOMs do not suffer from such a problem and exhibit behaviours such as aggregation-induced emission (AIE) or aggregation-enhanced emission (AEE). This property alone expands the utility and interestingly opens windows into their fundamental photophysical mechanisms.<sup>31</sup> The use of luminescent materials has been part and parcel of human ingenuity-from their first operational stages in phosphorescent and fluorescent systems. However, with the current trend on organic molecules that emit light in the solid state, this is a development relatively recently noted. This is mainly based on the premium demand for light-weight, flexible, and energy-efficient optoelectronic devices. Organic molecules, with

their structural diversity and tunability, are emerging as the ideal candidates for achieving these goals. They can form films, crystals, or powders without sacrificing luminescence efficiency. Organic molecules therefore surpass their inorganic counterparts in specific applications.<sup>32-33</sup>

Organic solid-state emissive materials have gained immense interest of late due to their outstanding optoelectronic properties, which resulted in the successful commercialization of organic electronics. However, attainment of highly efficient solid-state emission, or fluorescence, from organic chromophores is quite challenging due to molecular aggregation that causes quenching of emission. However, several approaches have been devised to obtain efficient fluorescence emission in the solid state by suppressing the undesired molecular aggregation.<sup>34</sup> At the outset, the review provides a brief summary of various designs and strategies of molecular building blocks for the preparation of solid-state emissive organic chromophores. In the many strategies, there is a focus on either partial or complete twisting of molecular building blocks, introduction of bulky substituents, or using a donor–acceptor type system, which can efficiently mitigate the intermolecular p–p stacking interaction and yield fluorescence emission in the solid state with high quantum yield. In this context, tuning and control of the fluorescence properties based on a single molecular building block is attractive to realize multicoloured emission and more advantageous for blending of different fluorescent materials in light emitting devices. Besides this many organic compounds can emit light not only from singlet excited states but also from triplet excited states. This phenomenon is known as room-temperature phosphorescence (RTP).<sup>35</sup>

### 1.5: Applications of Solid-State emissive molecules

The exceptionally outstanding photoluminescent properties of SSOMs—very high quantum efficiencies and significant luminescence in the aggregated or solid state—have led to considerable breakthroughs in several scientific and technological disciplines. The diversity of their applications ranges from optoelectronics to medicine. The following sections expand on these areas in depth, focusing on the advantages introduced within them and very recent developments.

#### 1. OLEDs

SSOMs have been widely recognized as utility materials in OLED synthesis. OLEDs form the nucleus of modern display and lighting technologies.

**Efficiency and Stability:** In OLEDs, SSOMs that have AIE or AEE properties are extremely desirable because they exhibit excellent quantum yields in the solid state—that is, they escape the common ACQ effect. It leads to bright, efficient light emission. The emission color of SSOMs is modulated through molecular modifications for bright, highly reproducible display devices.

Multi-color white OLEDs are currently being achieved by combining two or more different SSOMs with complementary emission spectra, which play a fundamental role in their lighting applications.

#### Thin-Film Flexibility

SSOMs can be fabricated into stable thin films on flexible substrates, positioning them well for future flexible and foldable display applications.

**Recent Advancements:** Recent studies have been carried out on the areas of thermally activated delayed fluorescence emitters and hybridized local and charge-transfer states that reduce energy losses in order to increase the internal quantum efficiency of OLEDs.

#### 2. Detection and Sensing

SSOMs have proved to be a high-power tool for sensing and detection due to their sensitivity towards the external perturbative factors and their effectiveness in being operated in the solid state.

- **Chemical Sensing**  
SSOMs exhibit an alteration in fluorescent intensity, color or lifetime upon contact with some target analytes such as gases, ions or small organic molecules. Such analytes comprise of:  
Detecting toxic gases such as ammonia or nitrogen oxides.

Environmental monitoring: The detection of metal ions, such as  $\text{Hg}^{2+}$  or  $\text{Fe}^{3+}$ . [36]

- **Biological Application**  
Biocompatibility is imparted to the SSOM wherein commutation tolerance of biological molecules like glucose, proteins, or DNA is gained. In this 'turn-on' effect fluorescence with associated molecular interaction very high sensitivity and selectivity is achieved.
- **Mechanofluorochromism**  
SSOMs with mechanofluorochromic properties respond to external mechanical forces like grinding or pressure through a change in emission color or intensity. Such behavior is attributed to applications in the detection of stress in materials, as well as in tamper-evident packaging.<sup>37</sup>

### 3. Bioimaging and Theragnostic

SSOMs exhibit crucial applications in the biomedical field, especially in the framework of bioimaging and theragnostic which is the trend today between therapy and diagnostics.

#### • Fluorescence Bioimaging

Solid-state emitters are good biological imaging agents because of excellent photostability, low cytotoxicity, and high luminescence in aqueous or aggregated environments.<sup>38</sup>

Applications in live-cell imaging, visualization of tumors, and tracking of biological processes.

#### • Theragnostic Agents

SSOMs can be multifunctional imaging agents and therapeutic tools. For instance, some SSOMs show photodynamic therapy capability. These can produce reactive oxygen species upon the irradiation of light to induce cell death to cancer cells while also enabling the imaging of a tumor.

#### • Recent Advances

Near-infrared (NIR) emissive SSOMs which are capable of more penetration into tissue depth for imaging applications. Dual-mode imaging agents that have fluorescence and MRI.

### 4. Optical Devices and Lasers

The highly intense solid-state luminescence of SSOMs is used in optical devices and laser applications.

#### • Organic Lasers

SSOMs are used as gain media in organic lasers due to their large photoluminescence quantum yields and tunable wavelengths of emission. The applicative fields range from medical diagnostics to optical communications. Waveguides and Optical Circuits High refractive index efficient luminescence materials are being used for interconnecting optical circuits to process signals and light amplification. [39]

#### Smart Windows and Displays:-

SSOMs with switchable luminescence properties are designed for smart windows, which change transparency or color in response to external stimuli to add energy efficiency to buildings.

## Chapter-2: EXPERIMENTAL STUDIES

### 2.1: Methods and Materials

We carried out two reactions for the synthesis of two Schiff bases.

#### For Reaction 1st

Chemicals: Sulphanilamide (99% from Sigma-Aldrich) [IUPAC Name:( 4-aminobenzenesulfamide)] and 4-(dimethylaminobenzaldehyde) (99% from Sigma-Aldrich) were used as the starting material (reactant) for this reaction. Distilled methanol and water were used in Schiff base reaction. The Schiff bases were prepared by mechano-grinding method and then the product was purified with the help of distilled Methanol.

### For Reaction 2nd:

Chemicals: Sulphanilamide (99% from Sigma-Aldrich) [IUPAC Name:( 4-aminobenzenesulfamide)] and 4-(diethylamino benzaldehyde) (99% from Sigma-Aldrich) were used as the starting material (reactant) for this reaction. Distilled methanol and water were used in Schiff base reaction. The Schiff bases were prepared by mechano-grinding method and then the product was purified with the help of distilled Methanol.

Melting points were measured on the MP70 melting point system capillary apparatus (Mettler Toledo) with closed-end capillaries. Infrared spectroscopic data of the Schiff base and its crystals are recorded by using an Agilent Technologies Cary 630 FT-IR (4000 – 400 cm<sup>-1</sup>) spectrometer. DR-UV studies, absorbance and reflectance spectra were recorded on Shimadzu 2600 spectrometer in BaSO<sub>4</sub> medium as reference. The fluorescence emission spectra were recorded on a Shimadzu RF-5301-PC spectrophotometer with varying exciting wavelengths in the solid phases. The thermogravimetric analysis of the samples was carried out on a thermal analyser-STA (LINSEIS, USA 6807/8835/16) by using an alumina crucible with a heating rate of 10 °C.

#### 2.2.1: Synthesis of Schiff base (HI-01)

For this reaction we take Sulfanilamide (0.344mg) and 4- dimethylaminobenzaldehyde (0.298mg), Scthiometric ratio 2:2 in Mortar and Pestle for grinding. After grinding for few minutes, a yellow product was obtained which was filtered using methanol. Few drops of Acetic acid were used as catalyst to carry out this reaction.

#### 2.2.2: Synthesis of Schiff base (HI-02)

For this reaction we take Sulfanilamide (0.344mg) and 4- diethylaminobenzaldehyde (0.254mg) Scthiometric ratio 2:2 in Mortar and Pestle for grinding. After grinding for few minutes, a deep greenish product was obtained which was filtered using methanol. Few drops of Acetic acid were used as catalyst to carry out this reaction.

### 2.3: Characterizations

**2.3.1: Melting point:** Melting points were determined on the MP70 melting point system capillary apparatus (Mettler Toledo) in closed-end capillaries. The melting point of HI-01 and HI-02, were recorded as 206-208°C and 100-102 °C respectively.

**2.3.2: FT-IR spectroscopy:** The Schiff base (HI-01 and HI-02) was initially confirmed by IR-spectroscopy. The synthesized Schiff base and exhibited different peaks in the FT-IR spectrum when compared to that of precursor materials that confirms to their formation.

**2.3.3: Thermal analysis:** Thermo-gravimetric analysis was performed on a thermal analyzer-STA (LINSEIS, USA 6807/8835/16) using an alumina crucible. A sample Of 15-20 mg of product HI-01 and HI-02 was placed in an aluminum pan and heated at the rate of 10°/min under nitrogen atmosphere.

**2.3.4: Characterization of photophysical properties:** Absorption spectra were collected on Shimadzu 2600 spectrometer in a BaSO<sub>4</sub> medium. Solid state Fluorescence emission spectra were recorded on a Shimadzu RF-5301-PC spectrophotometer with different exciting wavelengths.

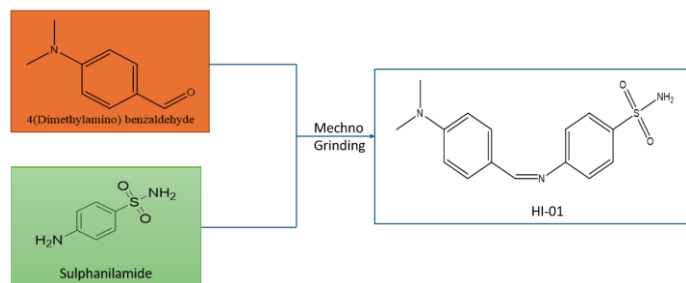
### 2.4 Properties

**2.4.1: Vapochromic Studies:** Vapochromic test of HI-01 was carried out at room temperature by exposing the compound to volatile organic vapors of HCl and HNO<sub>3</sub>, i.e., HI-01 showing different colors upon HCl and HNO<sub>3</sub> exposure. HI-01 at room temperature was kept on 100 mL beaker containing HCl and HNO<sub>3</sub> in it and HCl and HNO<sub>3</sub> fumes were given to HI-01(10 mg) of the compound, for 24 hours, the 100mL beaker was covered by 500mL beaker the HI-01 which was greenish yellow in color upon vapochromism changed color to red color and the emission was quenched.

**2.4.2: Thin film Studies:** Thin films were studied using UV-visible and emission spectroscopy of HI-01 in the liquid phase. Four polar aprotic solvents, i.e., THF, ACN and polar protic solvent, i.e., methanol and ethanol were used to study the mechanism of thin films.

### Chapter-3: RESULTS AND DISCUSSION

**Objective:** Synthesis of Schiff base with solid state emission was targeted and the design was based on crystal engineering principles. The solid-state emissive Schiff bases were studied to understand their property correlations and possible applications.



Scheme 1: Synthesis of HI-01

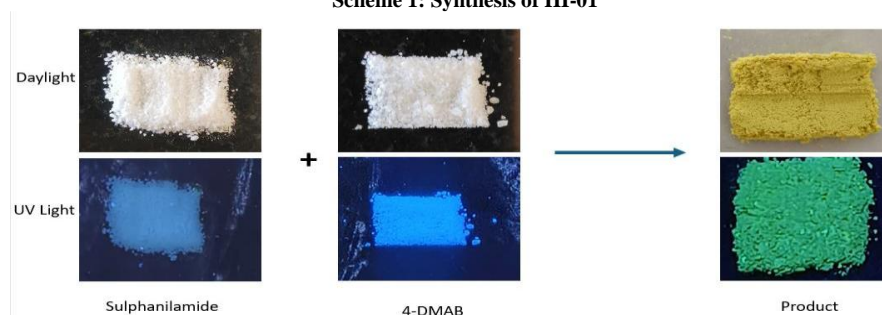
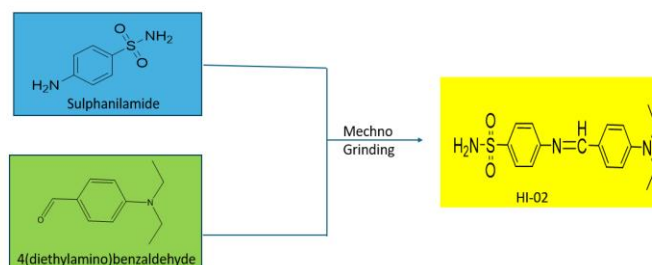


Figure 3.1: Optical images of HI-01 observed under daylight and UV-light



Scheme 2: Synthesis of HI-02

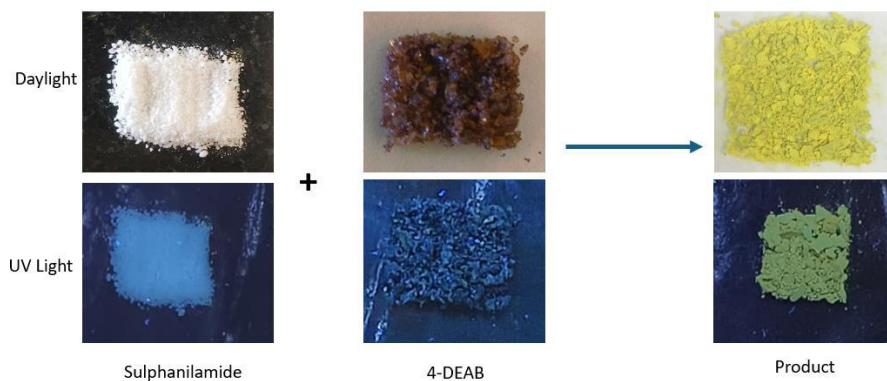


Figure 3.1: Optical images of HI-01 observed under daylight and UV-light

### 3.1: FT-IR analysis of Schiff-base (HI-01)

The yellow Schiff base was obtained by mechano-grinding precursors. The preliminary studies to characterize the Schiff base was done through Agilent Technologies Cary 630 FT-IR (4000–400  $\text{cm}^{-1}$ ) spectrometer.

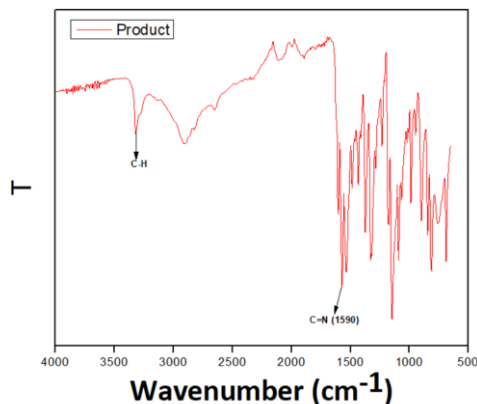


Figure 3.3: FT-IR spectra of HI-01(Schiff base) taken in neat form

The preliminary studies to characterize the Schiff base were done through Agilent Technologies Cary 630 FT-IR (4000-400  $\text{cm}^{-1}$ ) spectrometer. From the graph it can be seen that the peak observed around 3200 $\text{cm}^{-1}$  confirms the presence of C-H and the peak observed at 1590  $\text{cm}^{-1}$  confirms the presence of C=N, that actually validates the confirmation of our product HI-01 (Product).

### 3.2: TGA analysis of HI-01:

The TGA plot indicate that the thermal stability of product gets enhanced due to covalent bond formation compared to their precursors. The molecules are stable up to 300°C beyond which the decomposition (Weight loss) of organic moieties take place which can be perceived from the dips in the TGA curve.

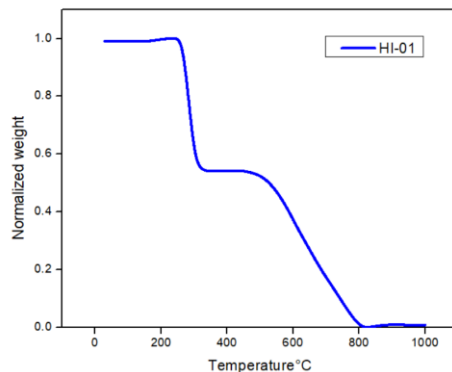


Figure 3.4: TGA plot of HI-01

### 3.3: Solid-state optical properties of HI-01

The appearance of intense yellow color in the HI-01 led us to investigate the optical properties of the HI-01 compared with the precursors. Diffuse reflectance studies on HI-01 were performed using BaSO<sub>4</sub> discs. The absorption peaks of sulphanilamide in the UV-visible region can be attributed to  $\pi-\pi^*$  transition and  $n-\pi^*$  transitions. The  $\pi-\pi^*$  transition and  $n-\pi^*$  transitions in 4-DMAB appeared as intense absorption bands in the wavelength region of 200-400 nm. The Schiff base viz HI-01 prepared from sulfacetamide and 4-DMAB exhibited three different peaks in the wavelength region of 200-500nm i.e a red-shift (Bathochromic shift) in the absorption spectra of HI-01 was observed which was substantiated by the incipience of intense yellow color in the HI-01. The red shift i.e the broad peak observed in the wavelength region of 300-500nm can be attributed to charge transfer interactions.

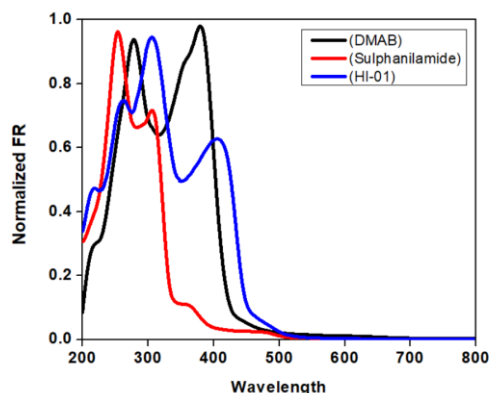


Figure 3.5: Diffuse-reflectance spectra of HI-01 collected in the form of BaSO<sub>4</sub> pellets.

### 3.4: Antioxidant Activity of HI-01:

It is the ability of a substance to neutralize free radicals or reactive oxygen species (ROS) that can cause oxidative stress in biological systems. Oxidative stress is associated with various diseases, including cancer, cardiovascular diseases, diabetes, and neurodegenerative disorders. Antioxidants can delay or inhibit the oxidation of biomolecules such as lipids, proteins, and DNA.

#### 3.4.1: DPPH Radical Scavenging Assay:

The DPPH (2,2-diphenyl-1-picrylhydrazyl) assay is one of the most commonly used methods for measuring antioxidant activity of samples. It is based on the reduction of the DPPH radical, a stable free radical that has a deep violet color, by antioxidants in the sample. When DPPH radicals are scavenged by antioxidants, the solution's color changes from violet to yellow, and this change is measured spectrophotometrically at 517 nm (Molyneux, 2004). The reduction in color intensity reflects the sample's ability to donate electrons or hydrogen atoms, indicating its radical-scavenging capacity.

**Advantages:** The DPPH assay is simple, quick, and requires only basic laboratory equipment. The Schiff base HI-01 was able to show the antioxidant activity of around 91%.

**3.5: Antimicrobial Activity:** - The zones of inhibition observed in the antimicrobial studies demonstrated concentration-dependent antimicrobial activity for the Schiff bases HI-01 and HI-02 derived from Sulphanilamide & 4-DMAB and Sulphanilamide & 4-DEAB.

1) 40 mg concentration HI-01

- Zone of Inhibition = 13 mm

2) 40 mg concentration HI-02

- Zone of Inhibition = 16 mm

Reference (streptomycin = 100 mg)

- Zone of inhibition = 17mm

#### Concentration-Dependent Efficacy:

The observed increase in the zone of inhibition with the Schiff base concentrations suggests an antimicrobial effect. This may indicate a dose-response relationship, with higher concentrations leading to increased efficacy against Bacillus.

- Comparison with references streptomycin

While the zones of inhibition for the Schiff bases are lower than the reference Streptomycin, the comparative

effectiveness indicates potential antimicrobial activity. The drug's efficacy, though lower, may still be relevant in certain contexts, especially considering the need for diverse antimicrobial agents.

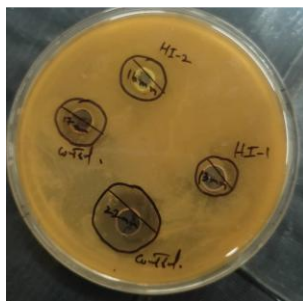


Figure 3.6: Antimicrobial activity with a zone of inhibition

### 3.6: Thin film studies

Thin films refer to thin layers of material deposited on a substrate with a thickness ranging from a few nanometers to several micrometers. Films based on these properties are becoming viable in various technological applications due to their unique properties and versatility. Thin films can be fabricated using numerous deposition techniques, including physical vapor deposition, chemical vapor deposition, sputtering, among others. Thin films are applied broadly in electronics, optics, coatings, and surface engineering. In electronics, thin films are used in semiconductor devices, integrated circuits, and thin-film transistors (TFTs). In optics, thin films are used in anti-reflection coatings, optical filters, and mirrors. In coatings, thin films impart protective layers with properties such as hardness, corrosion resistance, and wear resistance. In surface engineering, thin films are utilized in modifying surface properties, including adhesion, friction, as well as biocompatibility. Thin film properties can be suited to include optical, electrical, mechanical, and chemical characteristics through alteration in factors like deposition technique, deposition parameters, and material composition. These outstanding properties of thin films give them an essential place in a wide range of technological applications. Solid state Fluorescence emission spectra of thin films were recorded on an Agilent Cary Eclipse Fluorescence spectrophotometer with exciting Wavelength 485 nm.

HI-01 almost shows the same Emission in the same range (480-520) nm in solvents MeOH, EtOH, THF and ACN due to  $\pi-\pi^*$  and  $n-\pi^*$  transitions hence it does not show any shift viz bathochromic or hypsochromic.

## Chapter-4- CONCLUSION AND FUTURE PERSPECTIVE:

The applications of luminescent Schiff bases in crystal engineering make them of great importance due to their diverse applications, especially in optoelectronic devices, sensing, and photonics. Their tunable luminescence properties make them very promising for applications in different technological advancements. In conclusion, future prospects of such luminous Schiff bases in crystal engineering would be their further structural diversity investigation, the synthesis of new derivatives with adjusted properties, and integration into advanced materials for practical application in OLEDs, sensors, and biomedical imaging. Special attention in such research efforts might be on the photophysical properties of these molecules at the molecular level in order to tailor functionalities to meet certain applications. Astonishing changes in their respective Luminescent behavior by virtue of Mechanical Grinding and Heating hence can be used in various applications due to their Structural Diversity Luminescent Schiff bases exhibit a wide range of structural diversity, which enables the design and synthesis of molecules with tailored properties. This diversity allows for the exploration of different coordination geometries and packing motifs in the solid state, contributing to the field of crystal engineering. Tunable Luminescence The luminescent properties of Schiff bases can be finely tuned by modifying the molecular structure, such as the substituents on the aromatic rings or the central metal ion in metal-containing Schiff bases. This tunability is essential for customizing their optical properties for specific applications in optoelectronic devices and sensors. Crystal Engineering Applications Luminescent Schiff bases have found applications in crystal engineering for the construction of functional supramolecular architectures. Their ability to participate in various non-covalent interactions, such as hydrogen bonding,  $\pi-\pi$  stacking, and metal-ligand coordination, allows for the formation of diverse crystalline networks with specific optical properties. Future Prospects Synthesis of Novel Derivatives Continued research efforts will focus on synthesizing novel Schiff base derivatives with enhanced luminescent properties. This includes exploring new

synthetic methodologies, functionalizing the molecular structure with different electron-donating and electron-withdrawing groups, and investigating the incorporation of heteroatoms to modulate the electronic structure. Advanced Material Integration Luminescent Schiff bases hold promise for integration into advanced materials for various applications. Future research will explore their incorporation into organic light-emitting diodes (OLEDs), sensors for detecting analytes, and biomedical imaging agents for fluorescence microscopy and bioimaging. Photophysical Studies: Elaborative photophysical investigation on the molecular level, which deeply investigates the photo physics of luminescent Schiff bases, should represent an integral part of the understanding of their mechanisms of luminescence and establishment of optimized performance. Among others, this involves excited-state dynamics, emissive properties, and interactions with the surrounding environment in the solid state. Future advances in the strategy of crystal engineering will be addressed by designing and synthesizing luminescent Schiff base-based materials incorporating specific functionalities, which control the crystal packing arrangements by rational molecular design. The study of the role of crystal packing on optical properties will also continue. Emerging Applications With the field of luminescent materials continually growing, emerging applications for luminescent Schiff bases in photonics, information storage, even light-emitting devices will emerge; however, these will be quite demanding due to continued extensive interdisciplinary efforts to gap the basic understanding from the practical application process. Therefore, the future of luminescent Schiff bases in crystal engineering is toward the synthesis of novel derivatives, their incorporation into advanced materials, photophysical studies, advances in strategies on crystal engineering, and discovery of developing applications in diverse technological fields. Hence, continuing research efforts in such related areas are expected to continue unlocking the full potential of luminescent Schiff bases for a diverse range of practical applications.

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