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Synthesis and Characterization of Silver-Substituted Benzotriazole Coordination Polymer Network for the Inhibition of Disease-Causing Pathogens

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Abstract

We report the synthesis of a **silver–benzotriazole (SBT) coordination polymer network**, which facilitates the self-assembly of low molecular weight organic ligands into a metal–organic framework (MOF)-like structure. The compound was synthesized via a **wet precipitation method** and subsequently characterized using a suite of analytical techniques. **Powder X-ray diffraction (PXRD)** confirmed the formation and crystalline nature of the coordination polymer. **Fourier Transform Infrared Spectroscopy (FTIR)** revealed characteristic vibrational modes corresponding to benzotriazole ligands and their coordination to silver ions. **Scanning Electron Microscopy (SEM)** coupled with **Energy-Dispersive X-ray (EDX)** spectroscopy demonstrated that the particles exhibited agglomerated flake- and rod-like morphologies, and confirmed the presence of silver, nitrogen, and carbon in expected stoichiometric ratios. **UV–Visible spectroscopy** displayed prominent absorption peaks at 335 nm and 445 nm, indicative of surface plasmon resonance associated with silver nanoparticles and suggesting the presence of nanoscale features within the polymer network.The **biological activity** of the SBT complex was investigated, revealing potent antimicrobial effects against *Salmonella typhi* and *Staphylococcus aureus*. These results underscore the dual-functionality of the synthesized SBT coordination polymer as a

promising candidate for antimicrobial applications and highlight the therapeutic potential of metal–triazole complexes in modern medicinal chemistry.

Keywords: Silver benzotriazole (SBT); Antibacterial activity; Anticancer activity; Nanostructured materials

1. Introduction

Benzo-fused azoles represent a significant class of nitrogen-rich heterocyclic compounds with notable donor characteristics, making them of particular interest in pharmaceutical chemistry. Among them, azole derivatives have been clinically validated for their effectiveness in antimicrobial therapies [1]. Notably, **1,2,3-benzotriazole** was first proposed as a silver precipitating agent by **Remington and Moyer**, and later further investigated by **Tarasevich** [2]. Their studies also revealed that 1,2,3-benzotriazole can precipitate other metal ions such as **Cu (II)** and **Zn (II)**.**Silver** and its derivatives are extensively used in antibiotic formulations, particularly in topical creams, owing to their **exceptional antimicrobial properties** [3]. A prominent example is **silver sulfadiazine**, a widely used topical antimicrobial agent for treating burn wound infections [4,5]. Literature suggests that silver-based compounds possess strong antimicrobial activity against both **Gram-positive and Gram-negative bacteria**, which underscores their therapeutic potential.Integrating silver ions into **benzotriazole frameworks** can yield novel **coordination polymers (CPs)** or **metal–organic frameworks (MOFs)** with enhanced structural integrity, optical features, and biological activity. These hybrid materials are gaining attention for their potential in antimicrobial applications, attributed to the **synergistic effects** between the benzotriazole ligand and the silver center.With the **rapid emergence of antibiotic-resistant pathogens**, there is an urgent need to develop new classes of antimicrobial agents. In this context, **coordination polymers**, composed of metal ions and organic ligands, offer promising solutions due to their **structural tunability**, **functional versatility**, and **potential**

biomedical applications. Among various metal-based CPs, **silver-containing coordination networks** stand out because of silver's well-established **broad-spectrum antimicrobial efficacy** [6].This study focuses on the **synthesis and characterization of a silver-substituted benzotriazole coordination compound**, aiming to explore its potential as a multifunctional material. A comprehensive suite of characterization techniques—including **Fourier Transform Infrared (FTIR) spectroscopy**, **UV–Visible spectroscopy**, **Powder X-ray Diffraction (XRD)**, **Scanning Electron Microscopy (SEM)**, and **thermal analysis**—has been employed to probe the structural and functional attributes of the synthesized compound. The primary objective is to assess its suitability for **antimicrobial applications** and its relevance in the broader field of **materials science**.

2. Materials and methods

2.1 Chemicals

Analytical grade silver nitrate, **benzotriazole**, **ethylenediaminetetraacetic acid (EDTA)** and **ammonia solution** were procured from **Merck** and used as received, without any further purification. **Double-distilled water** was employed as the solvent in all experimental procedures.

2.2 Synthesis of SBT complex

An aqueous solution of **benzotriazole** (0.1 mol, 0.59 g in 50 mL distilled water), **silver nitrate** (0.1 mol, 0.84 g in 25 mL distilled water), and **disodium dihydrogen ethylenediaminetetraacetic acid (EDTA)** (8.49 g in 25 mL distilled water, equivalent to 10% of the benzotriazole concentration) were each prepared and stirred separately for 10 minutes at room temperature. Enough **ammonium hydroxide** was added to the EDTA solution to ensure complete dissolution, forming the **versanate solution**.

Subsequently, the silver nitrate solution was added **dropwise** to the versanate solution while maintaining the temperature at **60°C**. The mixture was adjusted to **neutral or slightly acidic**

pH using **dilute nitric acid**, and the temperature was maintained at 60°C. Following this, the benzotriazole solution was added dropwise, leading to the formation of a **white precipitate**.

The reaction mixture was stirred at **60°C for 15 minutes**, then allowed to cool to **room temperature**. The precipitate was filtered and **washed by centrifugation six times** using 10 mL of distilled water each time, then **dried at 110°C for 2 hours** to obtain a constant weight. The resulting **silver–benzotriazole complex** is referred to as **SBT**.

2.3 Characterisation

The **phase composition** of the crystalline **SBT complex** was analyzed using a **Rigaku Powder X-ray Diffractometer** equipped with a **CuKα radiation source** (λ = 1.5406 Å). To confirm the presence of functional groups, **Fourier Transform Infrared (FTIR) spectroscopy** was performed using a **Bruker Tensor 27 spectrometer** in the spectral range of **400–4000 cm^{-1}**, employing the **KBr pellet method**.The **surface morphology** and **elemental composition** of the synthesized sample were examined using a **Scanning Electron Microscope (SEM)** coupled with an **Energy Dispersive X-ray (EDX) spectrometer**. These analyses provided insights into the particle shape, size, and elemental distribution within the complex.Additionally, the **optical absorption characteristics** of the material were investigated using a **PerkinElmer LAMBDA 950 UV–VIS–NIR Spectrophotometer**, enabling the evaluation of electronic transitions and potential plasmonic behavior associated with the silver component.

3. Results and Discussions

3.1 Powder X-ray diffraction analysis

The crystalline structure and phase purity of the synthesized silver benzotriazole (SBT) coordination polymer were investigated using Powder X-ray Diffraction (PXRD) analysis. The PXRD pattern of the SBT complex is displayed in Figure 1. Obtained XRD pattern matched well with the previous report [7] which evident the formation of SBT. The diffraction pattern exhibits sharp and well-defined peaks, indicating the crystalline nature of

the material. Presence of broad x-ray peaks in the pattern indicates the existence of nanosized SBT grains. In comparing the experimental pattern (Fig. 1, top) with the reported one (Fig. 1, bottom).As per the previous report SBT correspond to the monoclinic crystal system with space group of $P2_1/c$ and the lattice parameters are a =14.8052 Å, b = 3.7498 Å and c =12.3495 Å. These parameters correlate well with the experimental data obtained in this study, further validating the identity of the compound. The observed diffraction pattern and corresponding peak positions suggest that the SBT compound is highly crystalline and phase pure, with no significant impurities or secondary phases detected.

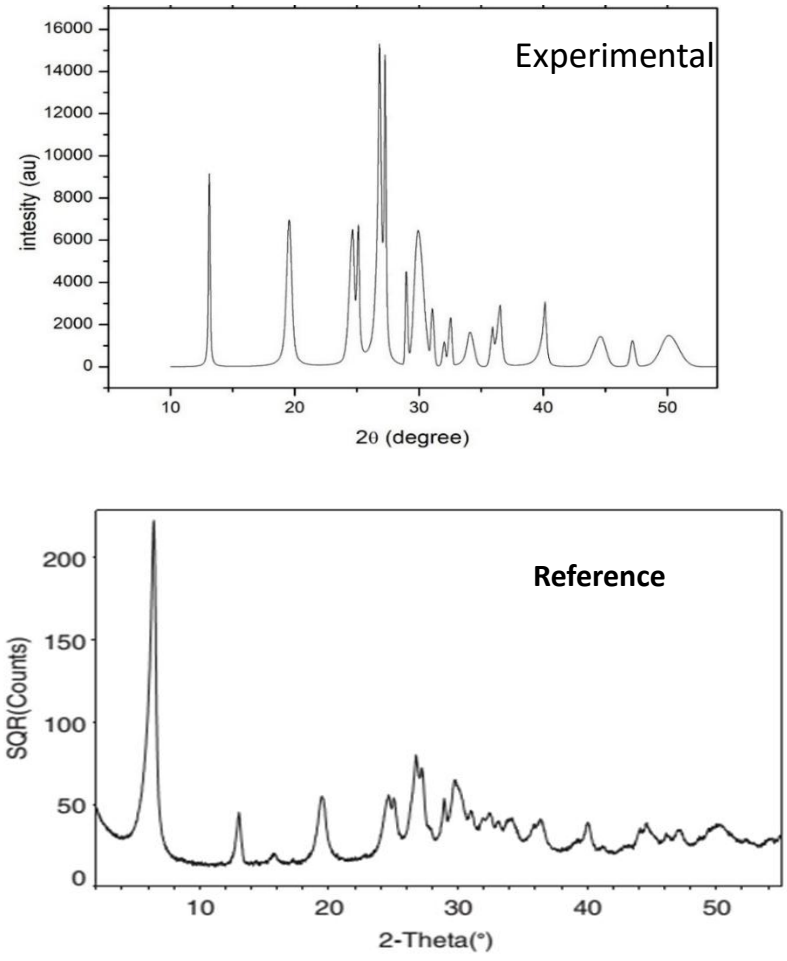


Figure 1: Powder X-Ray diffraction pattern of SBT compound

Compared to the reference pattern—presumably of pure benzotriazole or a structurally related compound—the experimental profile showed several distinct differences. While the

reference pattern displayed broader peaks of lower intensity, characteristic of a lower degree of crystallinity or possible amorphous nature, the experimental pattern revealed new, intense reflections, particularly between 20° and 35° 2θ. These newly emerged peaks suggest the successful formation of a novel crystalline phase, distinct from the parent ligand or any of its physical mixtures.The shift in peak positions and the appearance of additional reflections confirm that the SBT complex is not a mere physical blend but a chemically coordinated product, where silver ions have successfully interacted with benzotriazole ligands to form a coordination polymer network. The distinct peak pattern supports the formation of a new structural framework, most likely a metal-organic or coordination polymer, resulting from silver-ligand interactions. The PXRD analysis provides strong evidence for the successful synthesis of the SBT complex. The sharp diffraction peaks, in contrast with the broader peaks of the reference, validate the formation of a well-defined crystalline coordination compound. This structural distinction highlights the role of silver in organizing benzotriazole ligands into a crystalline polymeric network, thereby confirming the intended chemical modification and phase evolution. These results support the hypothesis that coordination between silver and benzotriazole can lead to new materials with distinct crystallographic and potentially functional properties.

3.2 FTIR spectral analysis

Fourier Transform Infrared (FT-IR) spectroscopy was employed to confirm the presence of functional groups and to investigate the bonding interactions in the synthesized silver benzotriazole (SBT) coordination complex. The FT-IR spectrum of the SBT compound is presented in Figure 2. The broad absorption band in the region of 2934–3034 cm^{-1} is attributed to the C–H stretching vibrations of the aromatic ring system, indicating the presence of the benzene moiety in the benzotriazole structure. The C–H in-plane and out-of-plane bending vibrations are observed in the 638–921 cm^{-1} range, which further confirms the

aromatic character of the ligand. A prominent absorption band at 1135 cm^{-1} corresponds to the C–N stretching vibration, which is a key indicator of the benzotriazole ring system. This band is crucial for confirming the triazole structure, as the C–N bond stretching occurs due to the electron delocalization within the aromatic nitrogen-containing ring. Another significant band is observed at 1487 cm^{-1}, which is assigned to the C=C stretching vibration of the aromatic ring. The presence of this band further supports the retention of aromaticity in the ligand structure after coordination with the silver ion.Additionally, the C–H out-of-plane bending vibrations appear clearly at 732 cm^{-1} and 789 cm^{-1}, which are typical for substituted aromatic rings. These bands provide further confirmation of the structural integrity of the benzotriazole framework within the complex.

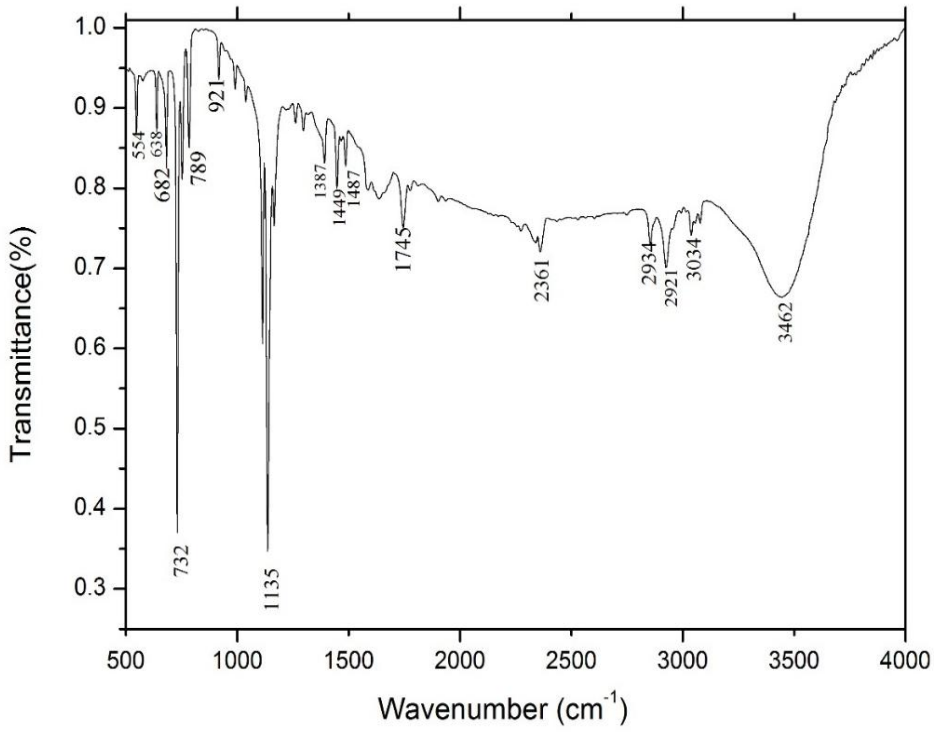


Figure 2: FTIR spectra of SBT

3.3 SEM WITH EDAX

The surface morphology and elemental composition of the synthesized silver benzotriazole (SBT) coordination polymer were examined using Scanning Electron

Microscopy (SEM) coupled with Energy Dispersive X-ray Spectroscopy (EDX). The SEM images, shown in Figure 3 (a–c), reveal that the particles are irregularly shaped and appear to be agglomerated. The morphology suggests that the SBT complex tends to form flake- or rod-like structures, which is characteristic of coordination polymers where extended frameworks and directional growth often lead to such morphologies. The average particle size was estimated to be approximately 70 nm, indicating that the synthesized SBT material falls within the nanostructured regime. In addition to morphological assessment, EDX analysis was performed to determine the elemental composition of the SBT complex. The EDX spectrum and elemental mapping images (Figure 3 d–h) confirm the presence of silver (Ag), nitrogen (N), and carbon (C) in the synthesized compound. The average elemental composition was found to be 6%, 3% and 91% for silver, nitrogen and carbon, respectively.

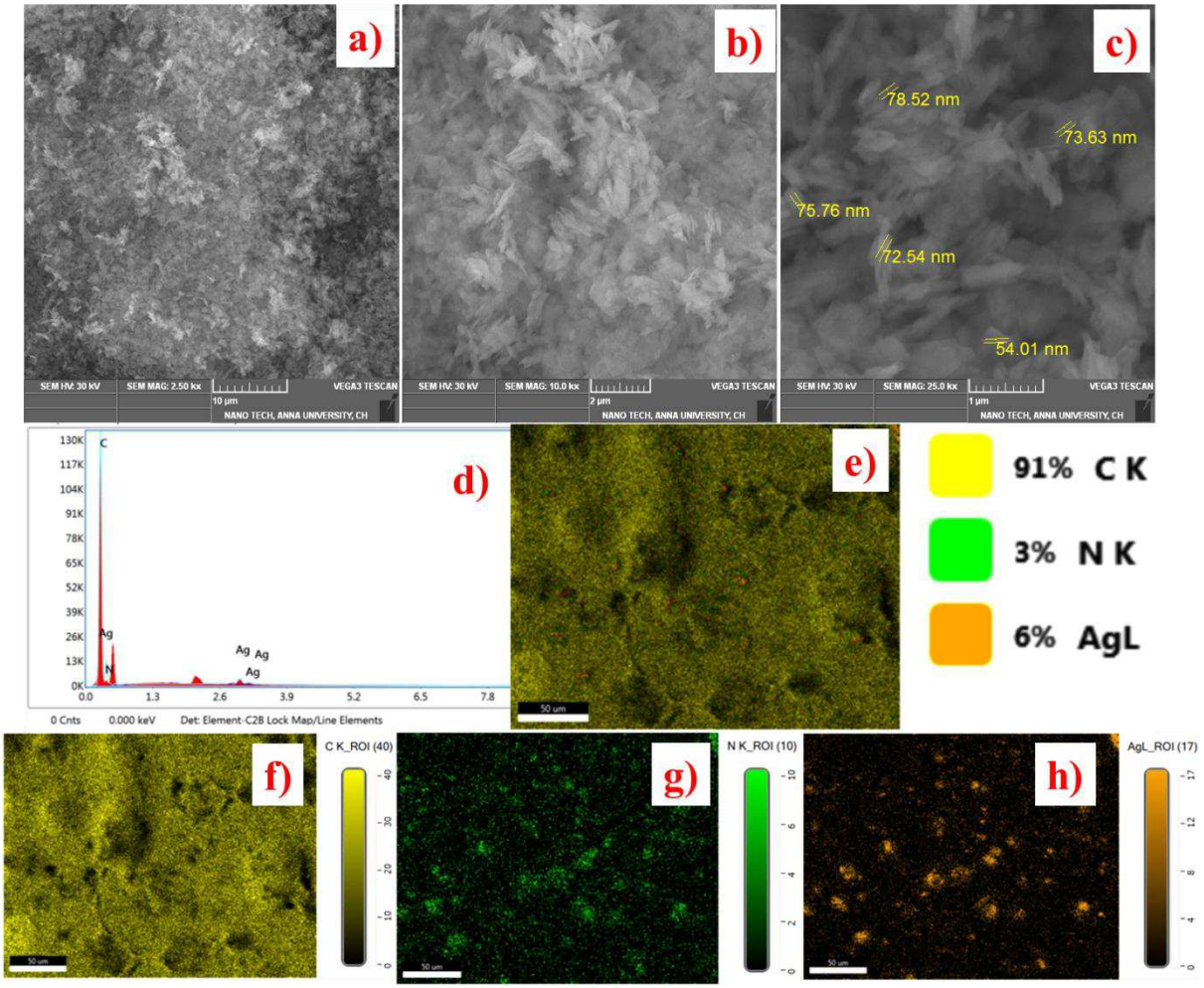


Figure 3: *a-c*) SEM images, d) EDX spectra and e-h) elemental mapping of SBT.

Table.1. weight percentage of elements in SBT compound

Element	Wt %
C K	60.04
N K	35.52
AgL	4.44

3.4 UV-Visible –NIR Spectrometer:

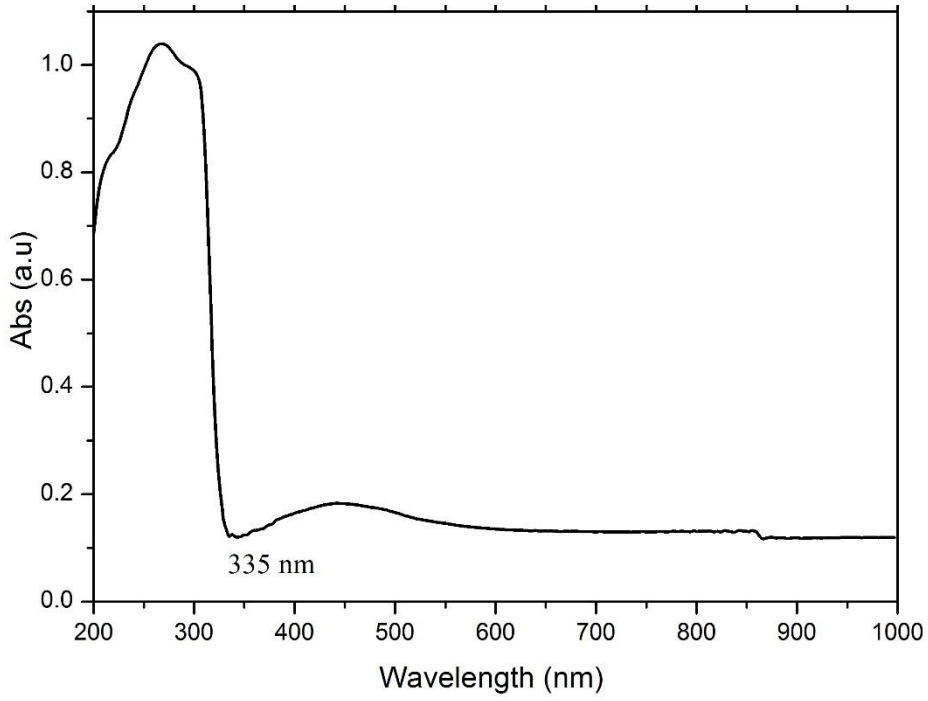
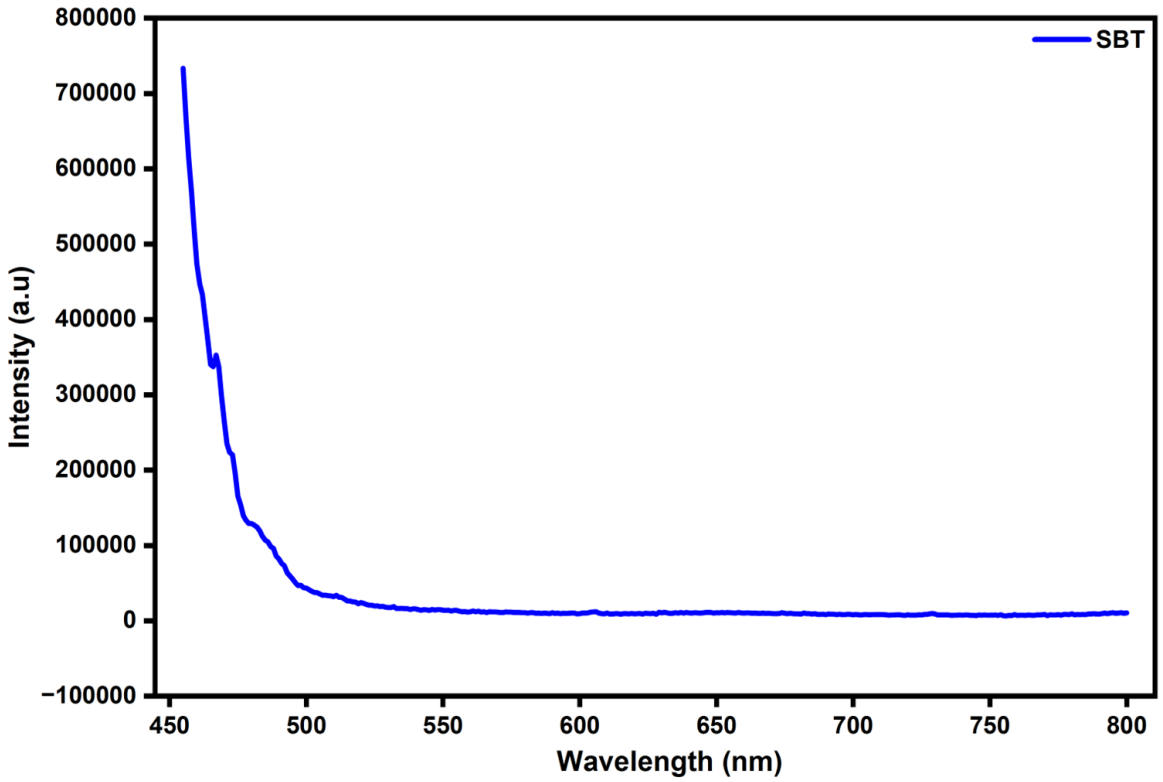


Figure 4: UV-Visible –NIR spectrum of SBT

UV-Visible–NIR spectroscopy was employed to investigate the optical properties and electronic transitions of the synthesized silver benzotriazole (SBT) coordination polymer. The absorption spectrum was recorded in the wavelength range of 200–1000 nm and the resulting spectrum is presented in Figure 4. The SBT complex exhibited two notable absorption features: one at 335 nm and another around 445 nm. The absorption peak observed at 335 nm is attributed to $\pi \rightarrow \pi^*$ electronic transitions within the aromatic system of the benzotriazole moiety. This is characteristic of conjugated organic systems and confirms the presence of aromatic rings and delocalized π-electron systems in the compound.

More significantly, the broad hump around 445 nm is indicative of the surface plasmon resonance (SPR) of silver nanoparticles or silver ions dispersed in the coordination polymer matrix.



3.5 photoluminescence studies

Photoluminescence (PL) spectroscopy was employed to investigate the electronic excitation behaviour and defect states of the synthesized silver benzotriazole (SBT) coordination polymer, as shown in Figure 5. PL analysis provides insights into the recombination of photoexcited charge carriers, which can be related to the material's electronic structure, purity, and potential optoelectronic or biological applications. The PL emission spectrum of the SBT complex was recorded at room temperature by exciting the sample at an appropriate excitation wavelength (typically ~325–375 nm for similar silver-organic systems). The resulting spectrum showed a broad emission band, commonly observed in the visible region, typically between 450–550 nm. This broad photoluminescence emission is attributed to the radiative recombination of electrons and holes trapped in surface or defect states of the material.

Figure 5: Photoluminescence studies SBT

3.6 TG/DSC studies

Thermogravimetric analysis (TGA) and Differential Scanning Calorimetry (DSC) were employed to investigate the thermal stability and decomposition pattern of the synthesized silver benzotriazole (SBT) coordination polymer. These thermal analytical techniques provide insight into the material's compositional integrity, phase transitions, and thermal decomposition behaviour under controlled heating conditions. The TGA curve of the SBT complex showed an initial minor weight loss below 150°C, attributed to the removal of adsorbed moisture or lattice water. A major weight loss occurred between 200°C and 400°C, corresponding to the decomposition of the organic benzotriazole ligand and partial breakdown of the coordination framework. The total weight loss in this region suggests the removal of organic moieties and the liberation of gaseous decomposition products. Simultaneously, the DSC curve displayed a broad endothermic peak in the same temperature range, confirming the occurrence of thermal decomposition. No sharp endothermic or exothermic peaks associated with crystalline melting or phase changes were observed, indicating the compound undergoes a gradual degradation rather than a sharp thermal transition. These results demonstrate that the SBT complex possesses moderate thermal stability, making it suitable for applications that do not involve exposure to extreme temperatures. The thermal behaviour supports the compound's structural integrity up to 200°C and validates its composition as a coordination polymer.

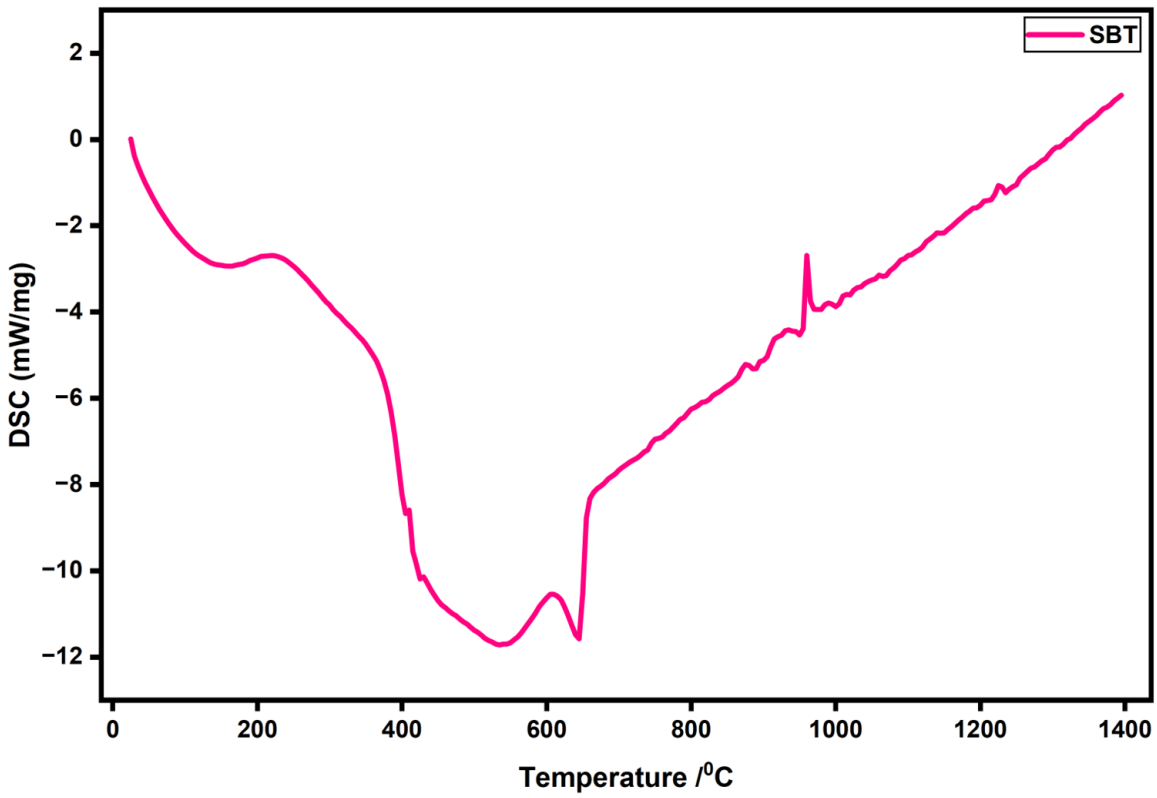


Figure 6: Differential Scanning Calorimetry analysis on SBT

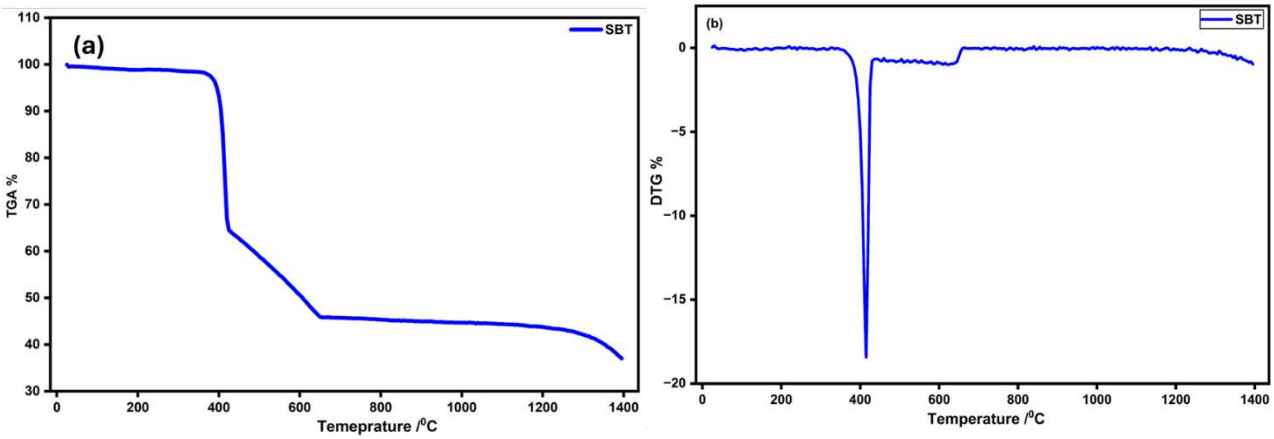


Figure 7: TGA and DTA analysis on SBT

4. ANTIMICROBIAL ACTIVITIES

The agar disc diffusion assay was used to determine the growth inhibition of bacteria and fungus by the sample (SBT compound). Muller-Hinton agar was prepared and poured into a sterile Petri dish plates and allowed to solidify. The overnight nutrient broth culture of gram-negative bacteria pseudomonas aeruginosa, gram-positive bacteria staphylococcus aureusand fungiCandida albicans, Aspergillusnigerspecies was inoculated in Mueller-Hinton

agar using sterile cotton swab. 500µg of the SBT sample were added to the sterile disc and incubated overnight at 37 °C. Antibacterial activity was recorded as growth of zone inhibition around the sterile disc.

s.no	Organism	STD(40µg) (Tetracyclene)	Sample (500µg) (SBT compound)
1.	***pseudomonas aeruginosa***	12mm	16mm
2.	***staphylococcus aureus***	34mm	15mm

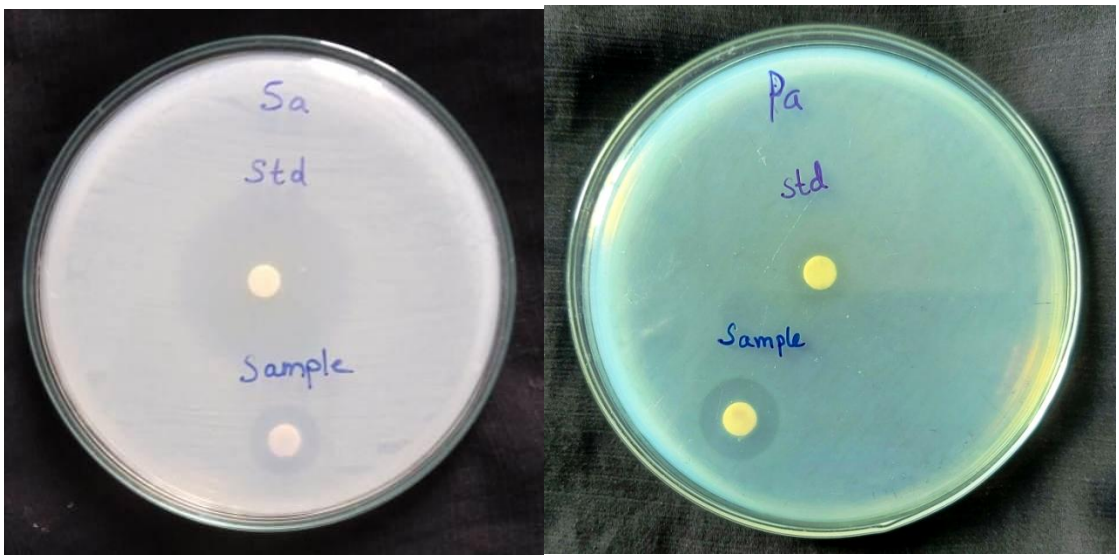


Fig.8. Anti-bacterial effect of SBT compound

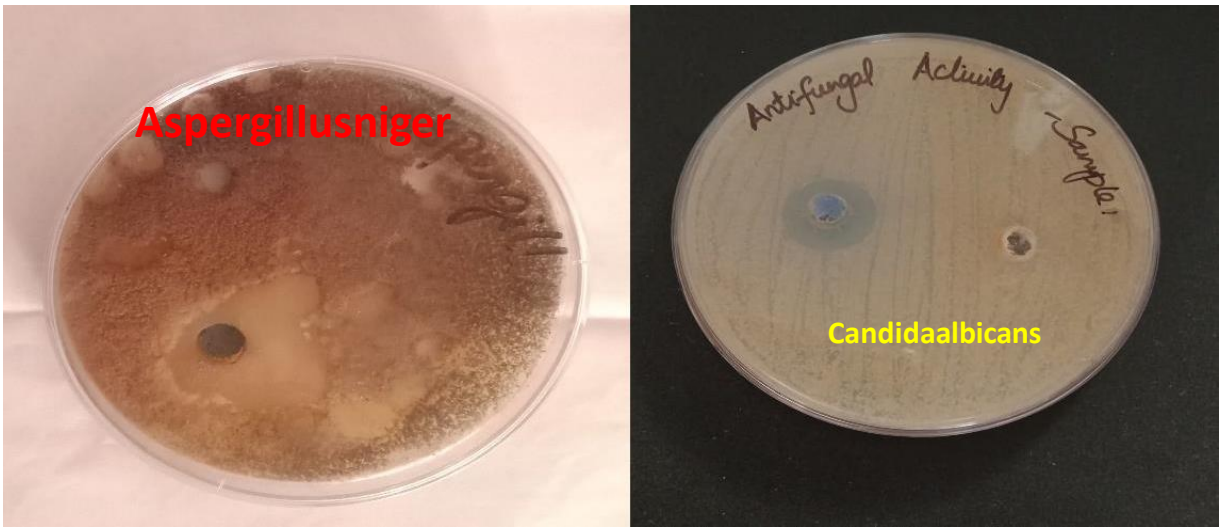


Fig.11. Anti-fungal of SBT compound

Sl.No	Organism	STD(40µg) Amphotericin B	Sample Zone of inhibition(500µg)CuBTA compound
1	Candidaalbicans	28mm	13.2mm
2	AspergillusNiger	30mm	23.5mm

4. Conclusion

Coordination compounds of silver with benzotriazole were synthesized by wet chemical precipitation method. The synthesised compound was characterised by various technique. The complex was confirmed by powder X-ray diffraction analysis. Functional groups were identified from FTIR spectral analysis. The EDX spectrum reveals presence of 6 % Silver, 3% Nitrogen and 91% Carbon was confirmed in SBT compound. From the SEM analysis, shape and size of SBT complex were identified. In the UV-Visible spectra, the cut off wavelength is found to be 335 and 445 nm. The biological activities of SBT molecule have also been exploredand was identified as potentialinhibitor for pseudomonas**aeruginosa** and **staphylococcus aureus**species. SBT may play an important role in the cytotoxic behaviour and exhibits good anticancer activity. These findings may guide to design new metal with triazole compounds are interesting biological activity.

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