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2 ND INTERNATIONAL SCIENCE, ENGINEERING AND TECHNOLOGY COLLOQUIUM



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PREFACE

Welcome to the 2nd International Science, Engineering and Technology Colloquium 2025 (ISETC 2025)!

It is with great pleasure that we present this year's colloquium, a distinguished gathering of scholars, researchers, and professionals dedicated to the advancement of applied sciences. Held virtually on 9th July 2025, ISETC 2025 serves as a platform to highlight cutting-edge research, foster meaningful networking, encourage collaborations, and explore innovative solutions to global challenges.

This year's theme, "The Power of Scientific Innovation: Intelligent Solutions for a Sustainable World" highlights our shared goal to solve global challenges through applied science. It celebrates innovation as a key to building a more sustainable and resilient future. We're proud to feature keynote speakers and presenters who bring fresh insights, bold ideas, and breakthroughs shaping tomorrow's world.

We would like to extend our heartfelt appreciation to the Faculty of Applied Sciences, Universiti Teknologi MARA, Perak Branch, Tapah Campus, for their outstanding support and assistance throughout the planning and execution of the event. Their dedication has been instrumental to the success of this colloquium. We would like to sincerely thank all participants and researchers for their valuable contributions. We also appreciate the reviewers for their careful evaluations and helpful feedback. Your hard work and support mean a lot to us.

As editors, we are proud to present this collection of proceedings. It is an honour to bring together the interesting and meaningful work of our speakers and authors. We hope the ideas shared will lead to new discoveries, encourage more research, and help solve global challenges through science and innovation.

Warm regards,

Dr. Emi Norzehan Mohamad Mahbob
Dr. Saiyidah Nafisah Hashim
Ms. Lili Widarti Zainuddin
Ms. Nurul Nazwa Mohammad
Ms. Rozaina Saleh

ISETC 2025 Proceedings Editors

SYNTHESIS AND FTIR CHARACTERIZATION OF 4-(DIPHENYLAMINO) BENZALDEHYDE-4-(3-NITROPHENYL) THIOSEMICARBAZONE

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Abstract: This study reports the successful synthesis and structural characterization of a new thiosemicarbazone derivative, 4-(diphenylamino)benzaldehyde-4-(3-nitrophenyl) thiosemicarbazone (Ligand 2), via a two-step condensation reaction. The first step involves reacting 3-nitrophenyl isothiocyanate with hydrazine hydrate to obtain 4-(3-nitrophenyl) thiosemicarbazide (Ligand 1), which is then condensed with 4-(diphenylamino) benzaldehyde to form Ligand 2. Structural confirmation was carried out using Fourier Transform Infrared (FTIR) spectroscopy, revealing characteristic vibrational peaks for azomethine (C=N) and thiocarbonyl (C=S) bonds. These spectral features confirm successful Schiff base formation and electronic modification. Based on similar findings in recent studies, this type of ligand shows promise for metal coordination and may contribute to the development of metallodrugs for anticancer and antimicrobial therapies (Fabra et al., 2024; Zahra et al., 2025).

***Keywords*:** *Thiosemicarbazone, metal complexation, Schiff Base, FTIR spectroscopy*

INTRODUCTION

Thiosemicarbazones (TSCs) are sulfur- and nitrogen-containing ligands capable of forming stable metal complexes, making them attractive in medicinal and environmental applications (Singh et al., 2023) However, designing TSC derivatives with enhanced selectivity and stability remains a challenge, particularly for cancer therapy and antimicrobial resistance. The objective of this study is to synthesize a novel TSC derivative, 4-(diphenylamino)benzaldehyde-4-(3-nitrophenyl) thiosemicarbazone, and to investigate how its electron-donating (diphenylamino) and electron-withdrawing (nitrophenyl) groups influence its metal coordination ability and potential biological activities. TSC-metal complexes have shown promising anticancer effects by inducing apoptosis, with copper-based complexes reported to inhibit tumor proliferation (Miglioli et al., 2024) and strong antibacterial properties through reactive oxygen species generation (Fabra et al., 2024). Furthermore, TSCs are useful in detecting fluoride and mercury ions, highlighting their environmental significance (Alharthy et al., 2023). The compound will be synthesized through a two-step condensation reaction and characterized by Fourier Transform Infrared (FTIR) spectroscopy to confirm key functional groups (C=N, C=S). The findings are expected to provide insight into how electronic substituents affect metal binding, aiding the development of selective metallodrugs and advancing TSC based sensing applications.

LITERATURE REVIEW

TSCs exhibit diverse bioactivities, including anticancer, antimicrobial, and diagnostic applications. Copper- and ruthenium-based TSC complexes inhibit tumor-promoting enzymes, induce apoptosis, and generate reactive oxygen species in cancer cells (Miglioli et al., 2024; Mohanty et al., 2025). Antimicrobial activity has been reported against multidrug-resistant pathogens, with copper-TSC complexes disrupting bacterial membranes (Fabra et al., 2024). Additionally, TSC-based hydrogels have shown promise for wound healing by releasing antimicrobial agents (Wang et al., 2024). In environmental applications, TSC derivatives act as fluorescent and colorimetric sensors for detecting fluoride ions and heavy metals (Alharthy et al., 2023; Özbek & Berkel, 2023). Their unique optical and solvatochromic properties also make them suitable for molecular switching, photopharmacology, and conductive self-healing materials (Kara et al., 2024; Silvarajoo et al., 2023). These studies highlight TSCs' versatility, reinforcing the

importance of designing new derivatives with enhanced metal coordination properties.

MATERIALS AND METHODS

Synthesis of 4-(Diphenylamino) benzaldehyde-4-(3-nitrophenyl) thiosemicarbazone (Ligand 2):

Preparation of Ligand 1 (4-(3-nitrophenyl) thiosemicarbazide)

3-Nitrophenyl isothiocyanate (0.003 mol) and hydrazine hydrate (0.003 mol) were reacted in ethanol (10 mL) with triethylamine (0.003 mol) under reflux for 6 hours. The reaction mixture was cooled, and the precipitate was filtered and washed with cold ethanol.

Preparation of Ligand 2

Ligand 1 (0.0001 mol) and 4-(Diphenylamino) benzaldehyde (0.0001 mol) reacted in ethanol (10 mL) with glacial acetic acid (5 drops) under reflux for 5 hours. The yellow product was isolated by vacuum filtration and washed with ethanol.

Characterization

FTIR Spectroscopy: The functional groups of the synthesized compounds were analyzed using FTIR (PerkinElmer Spectrum Two, 400–4000 cm^{-1}) to confirm the formation of key groups such as azomethine (C=N) and thiocarbonyl (C=S).

RESULTS

Synthesis and Yield

Ligand 1 (4-(3-nitrophenyl)thiosemicarbazide) was obtained with a yield of 7.91%. Ligand 2 (4-(Diphenylamino)benzaldehyde-4-(3-nitrophenyl)thiosemicarbazone) was synthesized with a yield of 92.72%. FTIR analysis confirmed the purity of both compounds, with no significant impurities detected.

FTIR Spectroscopic Analysis

Ligand 1: Exhibited characteristic peaks at 3349 cm^{-1} and 1623 cm^{-1} (N-H), 1251 cm^{-1} (C=S), 1525 cm^{-1} (NO_2) and C=C stretch at 1452 cm^{-1}.

Ligand 2: Displayed a redshift in C=N from 1623 cm^{-1} to 1584 cm^{-1}, confirming Schiff base formation, and a blueshift in C=S from 1251 cm^{-1} to 1215 cm^{-1}, indicating thione-thiol tautomerism. The nitro group and aromatic C=C stretches at 1525 cm^{-1} and 1491 cm^{-1} confirmed the electronic asymmetry in Ligand 2.

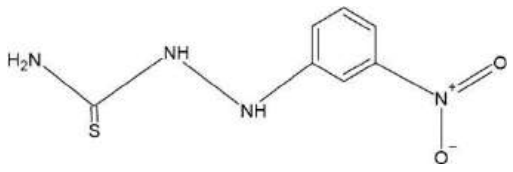


Figure 1. Structure of 4-(3-Nitrophenyl)thiosemicarbazide

Table 1. FTIR Data of 4-(3-Nitrophenyl)thiosemicarbazide (Ligand 1)

Wavenumber (cm^{-1})	Bond	Functional Group
3349.31	N-H	Amines
1622.74	N-H	Amines
1525.04	N=O (asymmetric)	Nitro group
1452.42	C=C	Aromatic ring
1250.63	C=S	Thioamide
1339.92	C-N	Amines

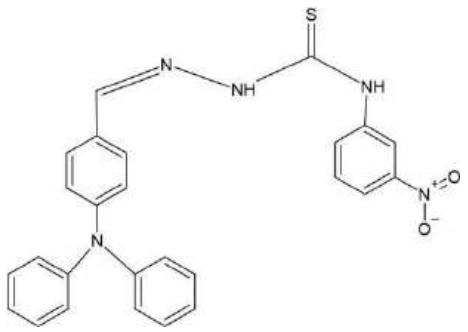


Figure 2. Structure of (4-(diphenylamino)benzaldehyde-4-(3-nitrophenyl)thiosemicarbazone)

Table 2. FTIR Data of (4-(diphenylamino)benzaldehyde-4-(3-nitrophenyl)thiosemicarbazone) (Ligand 2)

Wavenumber (cm^{-1})	Bond	Functional Group
1583.68	C=N	Azomethine
1558.15	N-H	Amines
1491.07	C=C	Aromatic rings
1270.00	C-N	Amines
1215.51	C=S	Thiocarbonyl

DISCUSSION/ANALYSIS

The FTIR analysis provided clear confirmation of the successful synthesis of both Ligand 1 (4-(3-nitrophenyl) thiosemicarbazide) and Ligand 2 (4-(diphenylamino) benzaldehyde-4-(3-nitrophenyl) thiosemicarbazone), highlighting significant structural differences between them. In Ligand 1, the presence of N-H stretching at 3349 cm^{-1} and bending at 1622 cm^{-1}, along with a C=S stretch at 1251 cm^{-1} and a C-N stretch at 1340 cm^{-1}, confirmed the intact thiosemicarbazide framework. In contrast, Ligand 2 exhibited disappearance of the N-H stretch and the appearance of a new C=N imine peak at 1584 cm^{-1}, verifying Schiff base formation through condensation with 4-(diphenylamino) benzaldehyde. Additionally, the C=S stretch shifted to 1215 cm^{-1} and the C-N stretch to 1270 cm^{-1} in Ligand 2, indicating electronic effects caused by conjugation and the influence of electron-donating and electron-withdrawing groups. These spectral shifts demonstrate that Ligand 2 underwent significant electronic modulation, which is crucial for enhancing its coordination ability with metal ions. This modulation is particularly relevant for the development of metallodrugs with therapeutic potential. While minor variations in the FTIR spectra may arise from residual solvents or incomplete reaction byproducts, the overall spectral data strongly support the successful synthesis and structural transformation of Ligand 2. These findings underscore the effectiveness of chemical modifications in tailoring ligand properties for targeted applications in medicinal chemistry

CONCLUSIONS

In conclusion, this study successfully synthesized and characterized a novel thiosemicarbazone (Ligand 2) via a two-step condensation reaction, confirmed through FTIR spectroscopy. Ligand 1 retained typical thiosemicarbazide peaks (N-H at 3349 cm^{-1}, C=S at 1251 cm^{-1}), while Ligand 2 showed clear Schiff base formation, evidenced by the C=N stretch at 1584 cm^{-1} and shifts in C=S (1215 cm^{-1}) and C-N (1270 cm^{-1}) (Imran et al., 2021; Fabra et al., 2024). These results confirm successful electronic modification, where diphenylamino and nitrophenyl substituents enhanced electronic asymmetry and potential for metal coordination, supporting its application in metallodrug development. Minor deviations may be due to residual solvents or incomplete reactions (Silvarajoo et al., 2023). Further studies using NMR, UV-Vis, CHNS analysis, and biological assays are recommended to explore its anticancer, antimicrobial, and metal-binding properties.

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