# INVESTIGATION OF THE METAL COMPLEXES OF ISOMERIC NAPHTHOIC ACID WITH BASE: SYNTHESIS, CRYSTAL STRUCTURE, AND ITS ENERGY APPLICATIONS

### **THESIS**

**Submitted to Bharathiar University** 

in partial fulfillment of the requirements for the award of the Degree of DOCTOR OF PHILOSOPHY

IN

**CHEMISTRY** 

**Submitted by** 

**M.SWATHIKA** 

Under the guidance of

Dr. N. ARUNADEVI, M.Sc., M.Phil., Ph.D.

**Assistant Professor** 



# DEPARTMENT OF CHEMISTRY PSGR KRISHNAMMAL COLLEGE FOR WOMEN

(Autonomous Institution – Affiliated to Bharathiar University)

**Coimbatore – 641004** 

Tamil Nadu, India

**SEPTEMBER 2023** 



## **CERTIFICATE**

This is to certify that the thesis, entitled "INVESTIGATION OF THE METAL COMPLEXES OF ISOMERIC NAPHTHOIC ACID WITH BASE: SYNTHESIS, CRYSTAL STRUCTURE, AND ITS ENERGY APPLICATIONS" submitted to the BHARATHIAR UNIVERSITY, in partial fulfillment of the requirements for the award of the Degree of DOCTOR OF PHILOSOPHY IN CHEMISTRY is a record of original research work done by Mrs. M. SWATHIKA during theperiod 2019 - 2023 of her research in the Department of Chemistry at PSGR KRISHNAMMAL COLLEGE FOR WOMEN, COIMBATORE, under my supervision and guidance and the thesis has not formed the basis for the award of any Degree / Diploma / Associateship / Fellowship or other similar title of any candidate of any University.

Place: COIMBATORE

Date: 23.09.2023

Signature of the Guide

Dr. N. ARUNA DEVI, M.Sc., M.Phil., Ph.D.,
Assistant Professor
Department of Chemistry
PSGR Krishnammal College for Women
Peelamedu, Colmbatore - 641 004.

Countersigned

**Head of the Department** 

Dr. D. NALINI M.Sc., M.Phil., B.Ed., MCA., Ph.D.
Associate Professor & Head
Department of Chemistry
PSGR Krishnammal College For Women
Peelamedu, Coimbatore - 641 004.

Dicolio

Principal
PRINCIPAL
PSGR KRISHNAMMAL COLLEGE FOR WOMEN
COMBATORE - 641 004



Declaration

## **DECLARATION**

I, M. SWATHIKA, hereby declare that the thesis entitled "INVESTIGATION OF THE METAL COMPLEXES OF ISOMERIC NAPHTHOIC ACID WITH SYNTHESIS, CRYSTAL STRUCTURE, AND ITS ENERGY APPLICATIONS" submitted to the BHARATHIAR UNIVERSITY, in partial fulfillment of the requirements for the award of the Degree of DOCTOR OF PHILOSOPHY IN CHEMISTRY is a record of original research work done by me during 2019- 2023 under the supervision and guidance of Dr. N. ARUNADEVI M.Sc., Assistant Professor. M.Phil., Ph.D., Department of Chemistry, KRISHNAMMAL COLLEGE FOR WOMEN, COIMBATORE, and it has not formed the basis for the award of any Degree/ Diploma/ Associateship/ Fellowship or other similar title to any candidate in any University.

Place: COIMBATORE

Date: 23.09.2023

Signature of the Candidate

Certificate of Genuineness of the Publication

## CERTIFICATE OF GENUINESS OF THE PUBLICATION

This is to certify that the Ph.D. candidate **M. SWATHIKA** working under my supervision has published a research article in the standard Scopus Journal named,

- 1. Surfaces and Interfaces, with Volume.24, page no.101094 and year of publication: 2021, published by Elsevier.
- 2. Journal of Molecular Structure, with Volume.1250, page no.131790 and year of publication: 2021, published by Elsevier.
- 3. RSC advances, with Volume.12, page no.14888-14901 and year of publication: 2022, published by Royal Society of Chemistry.
- 4. ECS Transactions, with Volume.107, page no.5763 and year of publication: 2022, published by IOP Publishing.
- 5. Luminescence, year of publication: 2022, published by Wiley luminescence
- 6. International Journal of Hydrogen Energy, year of publication: **2023**, published by Elsevier
- 7. Engineering, Science, and Sustainability, tear of Publication:**2023**, published by Taylor and Francis

The contents of the publication incorporate a part of the results presented in her thesis.

Signature of the Guide

Dr. N. ARUNA DEVI, M.Sc., M.Phil., Ph.D., Assistant Professor Department of Chemistry PSGR Krishnammal College for Women Peelamedu, Colmbatore - 641 004.

Countersigned

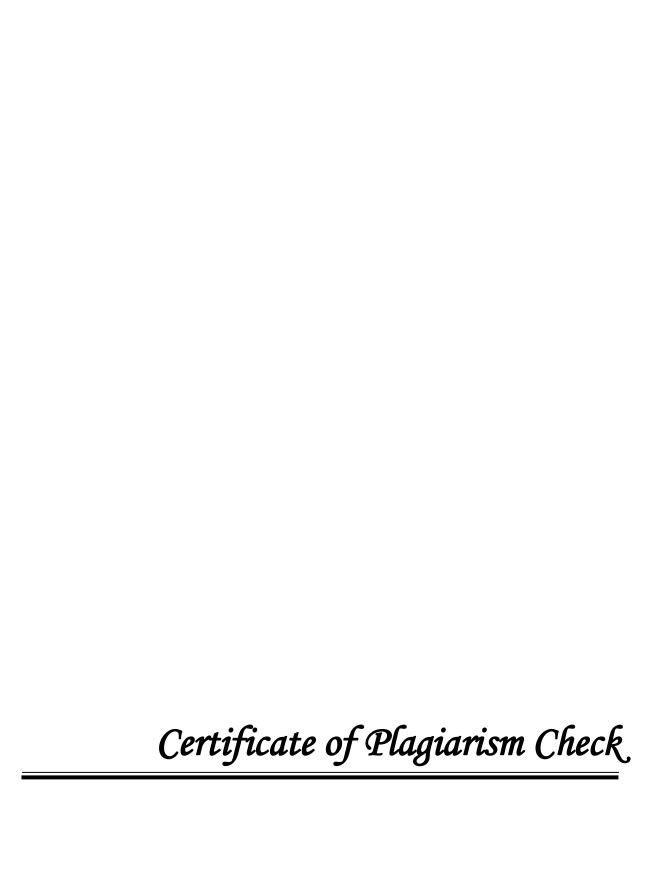
Head of the Department

Drogio

Dr. D. NALINI M.Sc., M.Phil., B.Ed., MCA., Ph.D.
Associate Professor & Head
Department of Chemistry
PSGR Krishnammal College For Women
Peelamedu, Coimbatore - 641 004.

Principal
PRINCIPAL
PSGR KRISHHARAMAL COLLEGE FOR WOMEN
COMMENTER: - 641 004







# பாரதியார் பல்கலைக்கழகம் BHARATHIAR UNIVERSITY COIMBATORE - 641 046, TAMILNADU, INDIA

State University | Re-Accredited with "A" Grade by NAAC | Ranked 15th among Indian Universities by MHRD-NIRF

# CERTIFICATE OF PLAGIARISM CHECK Name of the Research Scholar M. SWATHIKA 1 M.Phil., / Ph.D. Course of study 2 INVESTIGATION OF THE METAL COMPLEXES 3 Title of the Thesis / Dissertation OF ISOMERIC NAPHTHOIC ACID WITH BASE: SYNTHESIS, CRYSTAL STRUCTURE, AND ITS ENERGY APPLICATIONS Dr. N. Arunadevi Name of the Supervisor Department of chemistry PSGIR Krishnammal College for Women Department / Institution/ Research Centre % of Similarity of content Identified Acceptable Maximum Limit 7 10 % Software Used URKUND 22/09/2023 Date of verification

Report on plagiarism check, items with % of similarity is attached

Dr. N. ARUNA DEVI, M.Sc., M.Phil., Ph.D., Assistant Professor Department of Chemistry PSGR Krishnammal College for Women Peelamedu, Coimbatore - 641 004.

Head of the Department (Seal)

Dr. D. NALINI M.Sc., M.Phil., B.Ed., MCA., Ph.D.

Associate Professor & Head Department of Chemistry PSGR Krishnammal College For Women

Peelamedu, Coimbatore - 641 004.

Director i/c

Center for Research & Evaluation (BU) (Seal)

University Librarian

Arignar Anna Central Library **Bharathiar University** 

Coimbatore - 641 046.



#### Document Information

Analyzed document

Swathika. M.docx (D174350216)

Submitted

2023-09-22 08:02:00

Submitted by

Submitter email

buaacl.urkund@gmail.com

Similarity

2%

Analysis address

bhauni.urkund.buaacl.bhauni@analysis.urkund.com

#### Sources included in the report

### Bharathiar University, Coimbatore / Anu Priya. K.docx

SA

Document Anu Priya. K.docx (D44078272) Submitted by: bulib\_librarian@yahoo.co.in

Receiver: bulib\_librarian.bhauni@analysis.urkund.com

12

SA

C.Sharmila PhD Thesis Chemistry.pdf

Document C.Sharmila PhD Thesis Chemistry.pdf (D149204387)

品 1

#### **Entire Document**

CHAPTER I INTRODUCTION Nanotechnology refers to the utilization of technology on a minuscule scale, ranging from 1 to 100 nanometers, enabling the manipulation of matter at this level to create innovative materials and devices with exceptional properties. These advancements find practical applications in various fields, including medicine, electronics, energy, and the environment, leading to significant benefits for society. This rapidly emerging megatrend empowers scientists and engineers to employ individual atoms and molecules, forming functional structures that that have the potential to revolutionize numerous industries. 1.1 HISTORY OF NANOTECHNOLOGY

During an international conference on industrial production held in Tokyo in 1974, N. Taniguchi introduced the term "nanotechnology." This term described the precise manipulation of materials with nanometer precision and the study of nano-sized mechanisms. Subsequent to that period, from the late 1980s to the early 1990s, several significant greatly influenced. This led to a substantial increase in nanotechnological research and designs, resulting in a surge of publications on the subject and an expansion of practical applications. Consequently, there was significant increase in project financing and numerous organizations and countries became involved.

In 1991, the United States launched its inaugural nanotechnological program under the National Scientific Fund. Later, in 2001, the National Nanotechnological Initiative (NNI) was established with the primary goal of fostering collaboration among federal departments to prioritize nanotechnology development. The objective was to make nanotechnology the foundation for the USA's economy and national security in the first half of the 21st century. The term "nanometer" was first introduced by Richard Zsigmondy, He used a microscope ingeniously to measure the size of particles like gold colloids, coining the term "nanometer" for particle size characterization. In the 20th century, Richard Feynman, the Nobel Prize Laureate in physics in 1965, emerged as a visionary force. During the 1959 American Physical Society conference at Caltech, Feynman delivered a groundbreaking speech. In this speech, he presented the idea of manipulating matter at the atomic level, which laid the foundation for modern nanotechnology and opened up possibilities for technological advancements at the nanoscale.

Nanomaterials, also known as materials containing nanostructures, exist in various dimensions for their structural components. All these variations fall within the size range of 1-100 nm. When combined with polymers, biomolecules, or other nanostructured materials, these nanomaterials create nanocomposites, often leading to particle sizes larger than 100 nm. The exceptional physical and chemical characteristics of nanomaterials, , arise from their high surface-to-volume ratio.

University Librarian

Arignar Anna Central Library

Bharathiar University

Coimbatore - 641 046

Acknowledgement

## **ACKNOWLEDGEMENT**

First and foremost, praises and thanks to the **God**, the Almighty, for His showers of blessings throughout my research work to complete the research successfully.

I acknowledge my deep sense of gratitude towards the Management **Dr.** (Mrs.) S. Nirmala, M.B.A., M.Phil., Ph.D., P S G R Krishnammal College for Women, Coimbatore for providing the necessary facilities to carry out the dissertation in this reputed institution.

I express my profound gratitude to **Dr.** (**Mrs.**) **P. Meena.**, **M.Sc.**, **M.Phil.**, **Ph.D.**, Principal, PSGR Krishnammal College for Women, Coimbatore, for her constant support.

I express our heartfelt thanks to **Dr.** (**Mrs**). **D.** Nalini., **M.Sc.**, **M.Phil.**, **B.Ed.**, **MCA.**, **Ph.D.**, Assistant Professor & Head, Department of Chemistry, PSGR Krishnammal College for Women, Coimbatore, for her valuable encouragement throughout the period of our study.

I would like to express my deep and sincere gratitude to my research adviser, Dr. N. Arunadevi, M.Sc., M.Phil., Ph.D., Assistant Professor, Department of Chemistry, PSGR Krishnammal College for Women, for giving me the opportunity to do research and providing invaluable guidance throughout this research. Her dynamism, vision, sincerity and motivation have deeply inspired me. She has taught us the methodology to carry out the research and to present the research works as clearly as possible. It was a great privilege and honor to work and study under her guidance. I am grateful for what she has offered me. I would also like to thank her, for the empathy, and great sense of humor. Her guidance helped me in all the time of research and writing of this thesis. I could not have imagined having a better advisor for my Ph. D work. I thank her for having molded me to take up carrier in research field.

I would like to thank my research scholars Department of Chemistry, PSGR Krishnammal College for Women for their help and support.

I would like to thank all other faculty members of Department of Chemistry, PSGR Krishnammal College for Women for their timely help and guidance.

I would like to acknowledge the non-teaching staff members for their help.

I express my thanks to my friend **Sara** for their continuous help, kind constant support always by financial assistance during the duration of the study.

I would like to thank my lovable mom and dad Mr. R. Manoharan & M. Sathiya for their never ending effort to raise me and their keen interest in my education from early years right from my childhood leading up to the level of obtaining a Ph.D degree, which I feel is an act that cannot be express in words. My father is the one who raised me with her special care, everlasting love, and endless support in all dimensions of my studies. I express my love and gratitude to my beloved brother M. Kamatchi Nathan for their care and support in all pursuits. I also thank all the family members for their prayers, support and endless love. I would like to thank my special person my dearest sweartheart son T.S. Harshiv, who lost my motherly care and love during her childhood days. His sacrifice is thankfully acknowledged.

M.SWATHIKA

Abbreviations Used

# **ABBREVIATIONS USED**

mol --- mole

**g** --- gram

**GUA** --- Guanidine

**AMG** --- Aminoguanidine

NA --- Napthoic acid

**M.Pt** --- Melting

**bp.** --- Boiling point

M.wt --- Molecular weight

**Temp.** --- Temperature

Asym. --- Asymmetric stretching

Sym. --- Symmetric stretching

**Obsd.** --- Observed

Calcd. --- Calculated

**DTA** --- Differential thermal analysis

TG --- Thermogravimetry

(+) --- Endothermic transformation

(-) --- Exothermic transformation

**XRD** --- X-ray diffraction

**DFT** --- Density Functional Theory

**HOMO** --- Higher Occupied Molecular Orbit

**LUMO** --- Lower Occupied Molecular Orbit