

**CHALCONE DERIVATIVES AS ANTICORROSIVE ADDITIVES  
FOR MILD STEEL IN ACID MEDIUM: EXPERIMENTAL AND  
THEORETICAL INVESTIGATIONS**

**Thesis submitted to the Bharathiar University in partial fulfillment  
of the requirements for the award of the degree of**

***DOCTOR OF PHILOSOPHY IN  
CHEMISTRY***

By

**Mrs. N. ANUSUYA, M.Sc., M.Phil.,**

a doctoral fellow

Under the guidance of

**Dr. (Mrs.) SUBRAMANIAN CHITRA, M.Sc., M.Phil., Ph.D.,**

**Associate Professor**



**DEPARTMENT OF CHEMISTRY  
PSGR KRISHNAMMAL COLLEGE FOR WOMEN**

College with Potential for Excellence  
(An Autonomous Institution - Affiliated to Bharathiar University)  
(Reaccredited with 'A' Grade by NAAC)  
An ISO 9001: 2000 Certified Institution  
Coimbatore – 641 004

**MARCH - 2016**

## **CERTIFICATE**

This is to certify that the thesis entitled “**CHALCONE DERIVATIVES AS ANTICORROSIVE ADDITIVES FOR MILD STEEL IN ACID MEDIUM: EXPERIMENTAL AND THEORETICAL INVESTIGATIONS**” 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. **N. ANUSUYA M.Sc., M.Phil.**, during the period **2012 – 2016** 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 to any candidate of any University.

**Counter Signed**

**Signature of the Guide**

**Head of the Department**

**Principal**

## **DECLARATION**

I N. Anusuya hereby declare that the thesis, entitled “**CHALCONE DERIVATIVES AS ANTICORROSIVE ADDITIVES FOR MILD STEEL IN ACID MEDIUM: EXPERIMENTAL AND THEORETICAL INVESTIGATIONS**”, 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 and independent research work done by me during **2012 – 2016** under the Supervision and Guidance of **Dr. (Mrs.) SUBRAMANIAN CHITRA, M.Sc., M.Phil., Ph.D**, Associate professor, Department of **Chemistry** and it has not formed the basis for the award of any Degree / Diploma / Associate ship / Fellowship or other similar title to any candidate in any University.

**Signature of the Candidate**

## **CERTIFICATE OF GENUINNESS OF THE PUBLICATION**

This is to certify that the Ph.D. candidate **Mrs. N. ANUSUYA** working under my supervision has published a research article in the refereed SCI journal named **ORIENTAL JOURNAL OF CHEMISTRY** with Vol. No. **31(3)** Page Nos. **1741-1750** and year of publication **2015** published by **Oriental Scientific Publishing Company**. The content of the publication incorporates part of the results presented in her thesis.

**Countersigned**

**Principal**

**Research Supervisor**

## ACKNOWLEDGMENT

At the outset, I would like to express my sincere thank to the almighty God.

I acknowledge my profound sense of gratitude towards the management, the **Principal, Dr. S. Nirmala, MBA., M.Phil., Ph.D.**, and the **Secretary Dr. N. Yesodha Devi, M.Com., Ph.D.**, P.S.G.R. Krishnammal College for Women, Coimbatore, for providing the necessary infrastructure to carry out the dissertation in this reputed institution.

I am grateful and indebted to **Dr. K. Parameswari, M.Sc., M.Phil., Ph.D., Head of the Department of Chemistry**, for the valuable guidance and moral support to complete my project successfully.

Words are ineffable to my guide **Dr. Subramanian Chitra, M.Sc., M.Phil., Ph.D.**, Department of Chemistry, PSGR Krishnammal College for Women, Coimbatore for her advice during my doctoral research endeavor during the years. As my supervisor, she constantly forced me to remain focused on achieving my goal. Her observation and comments helped me to establish the overall direction of the research and to move forward expeditiously with investigation in depth. It could hardly have become possible for me to venture in the domain of research without her continuous guidance, patience, encouragement, motivation, enthusiasm, punctuality and parental care.

I express my heartfelt gratitude to all the teaching faculty of chemistry department for their help and moral support and for having inspiring me in various ways.

I wish to extend my heartfelt thanks to the **Director Y. Robinson**, RVS Technical Campus - Coimbatore for his constant support and encouragement throughout my research.

A special word of thanks to **Dr. P. Sounthari, M.Sc., M.Phil., Ph.D.**, Assistant Professor, Department of Chemistry, PSG College of Arts and Science and **Mrs. J. Saranya, M.Sc., M.Phil.**, Assistant Professor, Department of Chemistry, P.S.G.R. Krishnammal College for Women for the moral support and guidance rendered by them while carrying out this project.

I take this opportunity to thank my research colleagues, especially **E.Valarmathi, S. Jone Kirubavathy, V.P. Radha, G. Nirmala Devi** and all the research scholars in the

Department of Chemistry who supported and helped me during the course of my research work.

I take pleasure in thanking the **Non-teaching staff** of the Department of Chemistry for their help and co-operation.

I wish to earnestly thank my husband **Mr. S. Sekar**, who has given me his unequivocal support throughout and understanding of my goals and aspirations. I also appreciate my beloved daughter **S.S. Joshitha** for her love and co-operation.

I would like to express my deep sense of gratitude to my beloved parents and family members for their constant inspiration and encouragement.

**N. ANUSUYA**

## ABBREVIATIONS AND SYMBOLS

$\theta$	-	degree of surface coverage
$\sigma$ ohm/cm <sup>2</sup> /sec <sup>-1/2</sup>	-	Warburg coefficient
$\mu$	-	dipole moment
$\sigma$	-	global softness
$\chi$	-	electronegativity
$\eta$	-	global hardness
$\omega$	-	global electrophilicity
$\Delta E$	-	energy gap
$\Delta G^\circ$	-	standard free energy
$\Delta G_{\text{ads}}^\circ$	-	standard free energy of adsorption
$\Delta H^\circ$	-	standard enthalpy
$\Delta H_{\text{ads}}^\circ$	-	standard enthalpy of adsorption
$\Delta N$	-	fraction of electrons transferred
$\Delta S^\circ$	-	standard entropy
$\Delta S_{\text{ads}}^\circ$	-	standard entropy of adsorption
$\mu\text{A cm}^{-2}$	-	microamperes centimeter <sup>-2</sup>
$\mu\text{F cm}^{-2}$	-	microfarads centimeter <sup>-2</sup>
A	-	electron affinity
AAS	-	atomic absorption spectrophotometry
AFM	-	atomic force microscopy
$b_a, b_c$	-	anodic and cathodic Tafel slopes
$C_{\text{dl}}$	-	double layer capacitance
Con.	-	concentration
DFT	-	density functional theory
$E_a$	-	activation energy
$E_{\text{corr}}$	-	corrosion potential
EDS	-	energy dispersive X-ray spectroscopy
$f_{\text{max}}$	-	frequency maximum
FTIR	-	Fourier transform infrared spectroscopy

HOMO	-	highest occupied molecular orbital
I	-	ionization potential
$I_{\text{corr}}$	-	corrosion current
IE	-	inhibition efficiency
K (Degree)	-	absolute temperature
LUMO	-	lowest unoccupied molecular orbital
mM	-	millimole
$\text{mg lt}^{-1}$	-	milligram / liter
mpy	-	mils per year
$\text{g cm}^{-2} \text{h}^{-1}$	-	gram/centimeter <sup>2</sup> /hour
$\text{mV dec}^{-1}$	-	millivolts / decade
PZC	-	potential at zero charge
R	-	gas constant (8.314 K/J/mole)
$R_{\Omega}$	-	ohmic resistance
$R_{\text{ct}}$	-	charge transfer resistance
SEM	-	scanning electron microscope
TE	-	total energy
T°C	-	temperature in degree centigrade
T (K)	-	temperature in kelvin
Wt	-	weight
XRD	-	X-ray diffraction spectroscopy
$Z', Z''$	-	real and imaginary components of cell impedance