THE ELECTROCHEMICAL AND THEORETICAL STUDIES OF CORROSION INHIBITION OF ALUMINIUM IN ACIDIC AND BASIC SOLUTIONS BY BENZENE-1, 2, 4, 5-TETRACARBOXYLIC DIANHYDRIDE (PMDH)

ZOHREH SHAHNAVAZ

FACULTY OF SCIENCE

UNIVERSITY OF MALAYA

KUALA LUMPUR

2009

THE ELECTROCHEMICAL AND THEORETICAL STUDIES OF CORROSION INHIBITION OF ALUMINIUM IN ACIDIC AND BASIC SOLUTIONS BY BENZENE-1, 2, 4, 5-TETRACARBOXYLIC DIANHYDRIDE (PMDH)

ZOHREH SHAHNAVAZ

DISSERTATION SUBMITTED IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE DEGREE OF MASTER OF SCIENCE

FACULTY OF SCIENCE

UNIVERSITY OF MALAYA

KUALA LUMPUR

2009

To my parents,
sister and brothers.

For their love and prayers.

Abstract

The inhibitory activity of benzene -1, 2, 4, 5-tetracarboxylic dianhydride (pyromellitic dianhydride) on aluminium corrosion in hydrochloric acid (1.0 M HCl), sodium chloride (1.0 M NaCl) and potassium hydroxide (1.0 M KOH) was measured by means of electrochemical techniques such as electrochemical impedance spectroscopy (EIS) and polarization curves. The surface morphology was studied using scanning electron microscopy (SEM). The results indicate that benzene -1, 2, 4, 5-tetracarboxylic dianhydride suppress aluminium corrosion in these three media by its adsorption on the aluminium surface according to Langmuir adsorption isotherm. Potentiodynamic and EIS measurements indicate that the inhibition efficiency increases with the decrease in temperature and increase in the concentration of the inhibitor. On the other hand quantum chemical calculations show a correlation between molecular parameters and the corrosion behavior of PMDH.

ACKNOWLEDGEMENTS

I would like to express my extreme gratitude to both of my supervisors for their invaluable help during this project: Associate Professor Dr. Wan Jeffrey Basirun, who continuously shared his knowledge, advised and supported me all the way through and Associate Professor Dr. Shariffudin Mohd. Zain, for his sincere guidance, support and comments.

I would like to thank as well the PhD students Mehdi Ebadi and Mohammad Reza Mahmoudian for their experience was of great help to me.

I would like to express my thanks to all my friends for their help, moral support and memorable days we shared together.

I sincerely thank to my parents, my sister and my brothers who gave me so much support and encouragement throughout these years.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF SYMBOLS

F	: Faraday constant, 96485 C eqv^{-1}
R	: Gas constant, 8.314 J mol^{-1} K^{-1}
i	: Measured current density, A
i_{corr}	: Corrosion current density, A
n	: The number of electrons transferred in the anodic
$n´$	: The number of electrons transferred in the cathodic
β	: Potential drop coefficient
α	: Potential drop coefficient
T	: Absolute temperature, K
R_p	: Polarization Resistance, Ω
CR	: Corrosion Rate, mm/year
Z_{re}	: Frequency-dependent Real, Ω
Z_{im}	: Frequency-dependent Imaginary, Ω
$\hat{T}$	: Kinetic energy, 1 N. m
$\hat{V}$	: The Potential energy of the nuclear-electron attraction,1 N. m
$\hat{W}$	: The Electron-electron Repulsion
$\hat{H}$	: The Electronic Hamiltonian
ψ	: Electronic Wave Function
$E_{XC}[\rho]$	: Exchange-correlation functional
b_a	: Anodic Tafel slope

b_c : Cathodic Tafel slope

E_{corr} : Corrosion Potential, V

K_{ads} : Equilibrium Constants

C_{inh} : Inhibitor Concentration, M

θ : Surface Coverage Value

K : Adsorption Equilibrium Constant

ΔG_{ads} : Free Energy of adsorption

A : Plot of log Corrosion Rate

E_a : Activation Energy

ΔH^* : The Enthalpy of Activation

ΔS^* : The Entropy of Activation

h : Plank Constant, 6.626068×10^{-34} J.S

N : Avogadro's Number

C_{dl} : Double Layer Capacitance

R_s : Solution Resistance, Ω

η : Molecular Hardness

μ : Chemical Potential

LIST OF ABBREVIATIONS

PMDH	: Pyromellitic Dianhydride
EIS	: Electrochemical Impedance Spectroscopy
DFT	: Density Functional Theory
SHE	: Standard Hydrogen Electrode
HCl	: Hydrochloric Acid
Na_2SO_4	: Sodium Sulphate
NaCl	: Sodium Chloride
Al_2O_3	: Aluminium Oxide
$Al(OH)_3$	: Aluminium Hydroxide
AlO(OH)	: Aluminium Oxide Hydroxide
IE	: Inhibition Efficiency
LSV	: Linear Sweep Voltammetry
SEM	: Scanning Electron Microscopy
HF	: Hartree-Fock method
CI	: Configuration Interaction theory
PT	: Perturbation Theory
CC	: Coupled Cluster
LDA	: Local Density Approximation
GGA	: Generalized Gradient Approximation
STO	: Slater Type Orbitals
GTO	: Gaussian Type Orbitals

DZ	: Double Zeta
T Z	: Triple Zeta
KOH	: Potassium Hydroxide
SCE	: Saturated Calomel Electrode
NHE	: Normal Hydrogen Electrode
NaOH	: Sodium Hydroxide
HF	: High Frequency
IF	: Intermediate Frequency
LF	: Low Frequency
PCM	: Polarized Continuum Model
EDL	: Electric Double Layer
HOMO	: Highest Occupied Molecular Orbital
LUMO	:Lowest Unoccupied Molecular Orbital
IP	: Ionization Potential
EA	: Electron Affinity