

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

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**DISSERTATION SUBMITTED IN PARTIAL FULFILMENT OF THE
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KUALA LUMPUR**

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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.

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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^\ddagger	: The Enthalpy of Activation
ΔS^\ddagger	: 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 ₂ SO ₄	: Sodium Sulphate
NaCl	: Sodium Chloride
Al ₂ O 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