



UNIVERSITI
TEKNOLOGI
MARA

THE DOCTORAL RESEARCH ABSTRACTS

Volume: 9, Issue 9 April 2016

NINTH ISSUE

INSTITUTE of GRADUATE STUDIES

IGS Biannual Publication



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Title : Studies on the Adsorption and Corrosion Inhibition of Substituted Benzylidene Schiff Bases On Mild Steel In 1 M HCl

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The objective of this thesis is to investigate the performance of newly synthesized substituted benzylidene Schiff bases as corrosion inhibitors of mild steel in 1 M HCl at 25°C. To accomplish this intention, a series of (*E*)-*N*²-benzylidene-*N*⁴-phenylbenzene-1,4-diamine Schiff bases that contain different substituent groups at *para* position of benzylidene were synthesized and characterized via physical and spectroscopic analysis. The azomethine double bond (C=N) infrared spectra found for the Schiff bases are at around 1590-1604 cm⁻¹. From ¹H Nuclear Magnetic Spectroscopy (NMR) spectra, the azomethine proton (singlet) shifted in the range of δ 8.634-8.531 ppm, while the peaks at around δ 157.32-155.82 ppm found in ¹³C NMR spectra are assigned for azomethine carbon. The corrosion inhibition performance of *N*-phenyl-1,4-phenylenediamine (NPPD), (*E*)-*N*¹-benzylidene-*N*⁴-phenylbenzene-1,4-diamine (K1), *N*-[(*E*)-4-chlorobenzylidene]-*N*²-phenylbenzene-1,4-diamine (K2) and *N*-[(*E*)-4-methoxybenzylidene]-*N*²-phenylbenzene-1,4-diamine (K3) was measured in 1 M HCl using electrochemical methods which are polarization, Linear Polarization (LPR) and Electrochemical Impedance Spectroscopy (EIS). The analysis of substrate's surface *via* Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM) and X-ray Photoelectron Spectroscopy (XPS) was employed to determine the Schiff base adsorption behaviour on the surface of mild steel in the acidic solution. The electrochemical results revealed that the corrosion inhibition efficiencies of the Schiff bases are higher and achieved up to 96.0% as found for K2, thus more effective than the other Schiff base in the series, and the parent amine of NPPD. The adsorption of inhibitors at the metal-solution interface are well described

based on Langmuir adsorption isotherm because R^2 and slope values are almost to the value of 1. In further work, the temperature effect of Schiff bases in 1 M HCl also has been evaluated using polarization method. The inhibition efficiencies found for K2 inhibitor retains its great inhibitive effect and increase slightly until become almost constant at the highest temperature of 55°C. XPS measurements showed that studied Schiff bases mainly adsorbed *via* chemisorption interaction which involves coordination bond mainly electron donation from π electrons in the benzene ring and azomethine double to the empty orbital of metal. This is supported by ΔG_{ads} values which suggests the adsorption of Schiff base inhibitors on mild steel surface are due to the both combination of chemisorption and physisorption. The multilayers adsorption of inhibitors is due to subsequent layer physisorbed on the inner most (chemisorbed) layer via weak intermolecular hydrogen bonding of C-H- π between Schiff base molecules. The relationship between the corrosion inhibition efficiency with physicochemical and electronic properties of *N*-phenyl-1,4-phenylenediamine and Schiff bases was examined *via* density functional theory method. Theoretical results clearly shown that the corrosion inhibition efficiency of inhibitors are essentially depends on the frontier orbitals parameters as example by the increase of inhibition efficiency always directly related to the decrease of band gap energy between HOMO and LUMO. It is proven there is an electron transfer interaction among the Schiff base molecules with the active sites at the metal surface..