

CONTENTS

CHAPTER 1 INTRODUCTION	1-60
1. Introduction	1
1.1. Economic losses	1
1.2. General aspects of Corrosion	3
1.3. Corrosion problems in oil/petroleum industry	4
1.4. Acidizing treatment in oil wells	4
1.5. Classification of corrosion	5
1.5.1. Dry corrosion or chemical corrosion	5
1.5.2. Wet corrosion or electrochemical corrosion	6
(a) Anodic processes:	6
(a) Cathodic processes:	6
1.6. Common forms of corrosion	7
1.6.1. Uniform corrosion	7
1.6.2. Galvanic corrosion	7
1.6.3. Crevice corrosion	8
1.6.4. Pitting corrosion	8
1.6.5. Intergranular Corrosion	8
1.6.6. Stress Corrosion	8
1.6.7. Fretting corrosion	9
1.6.8. Corrosion fatigue	9
1.7. Factors affecting corrosion	10
1.7.1. Metal behavior	10
(a) Position in the galvanic series	10

(b) Relative areas of the anode and cathode	11
(c) Physical state	11
(d) Solubility of the corrosion products	11
1.8. Theories of Corrosion	11
(i) Homogeneous theory	11
(ii) Heterogeneous theory	12
(iii) Mixed Potential Theory	12
1.8.1. Thermodynamic aspects	13
1.8.2. Potential pH-diagram	14
1.8.3. Kinetic aspects - Polarization diagrams	17
1.8.3.1. Kinetic of equilibrium	17
1.8.3.2. Kinetics of polarization	17
1.8.3.3. Activation controlled polarization	18
1.8.3.4. Concentration polarization	19
1.9. CORROSION KINETICS	20
1.9.1 Graphical representation of kinetic data	20
1.9.2 Evans diagram	21
1.9.3. Mixed potential theory	23
1.9.4. Corrosion potential and current density	23
1.9.5. Tafel extrapolation method	25
1.10. Linear polarization methods	27
1.11. Electrochemical Impedance Spectroscopy (EIS)	28
1.12 Corrosion control methods	31
1.13. Corrosion Inhibitors	32
1.13.1. Definition of Inhibitor	32
1.13.2. Classification of Inhibitors	32
1.13.3. Environmental Conditions	33
1.13.4. Interface inhibitors	33

(a) Anodic Inhibitors	33
(b) Cathodic Inhibitors	34
(c) Mixed Inhibitor	36
(i) Inorganic inhibitors	37
(ii) Organic inhibitors	38
1.13.5. Interface inhibitors (Vapor phase)	38
1.14. Mechanism of corrosion inhibition in acid solution	39
1.15. Theories of inhibition	40
1.15.1. Adsorption Theory	40
(a) Adsorption Isotherms	40
(b) Adsorption of Inhibitor in acidic solution	41
1.15.2. Film Theory	42
1.15.3. Hydrogen Overvoltage	42
1.16. Application of Theoretical methods in Corrosion Inhibition Studies	42
1.16.1. Quantum chemical calculations	42
1.16.2. DFT based Quantum Chemical Parameters	43
(a) Atomic charges	44
(b) Molecular orbital energies and related parameters	44
(c) Dipole moment	45
(d) Fukui indices	46
1.17. Molecular dynamics simulations	46
1.18. Effect of inhibitors on corrosion processes	47
(a) Formation of diffusion layer	48
(b) Blocking of reaction sites	48
(c) Precipitation in the electrode reactions	48
1.19. Organic Compounds as Corrosion Inhibitors: Literature survey	48
1.20. The scope and importance of corrosion inhibition technology	60
1.21. Objective of present study	60

CHAPTER 2: EXPERIEMNTAL	61-80
2.1. Materials	61
2.1.1 Composition and dimensions of used Mild steel sample	61
2.1.2 Test solution	61
2.1.3 Inhibitors	61
2.2 Synthesis of inhibitors	62
2.3 Equipments and techniques used	72
2.3.1. Characterization of the Synthesized Compounds	72
(i) Determination of melting point	72
(ii) Spectroscopic characterization	72
2.3.2. Determination of corrosion rate and other related parameters	72
2.3.2.1 Weight loss method for determination of corrosion rate	72
2.3.2.2 Electrochemical measurements	73
2.3.2.2.1 Electrochemical impedance spectroscopy:	74
2.3.2.2.2 Potentiodynamic polarization:	75
2.4 Thermodynamic parameters	75
2.4.1 Activation energy:	75
2.4.2 Free energy of adsorption:	76
2.5 Scanning electron microscopy (SEM)	76
2.6 Atomic force microscopy (AFM)	77
2.7 Quantum chemical calculations	77
2.8 Monte Carlo simulations	79

CHAPTER 3: RESULTS AND DISCUSIONS	81-196
3.1 Pyrano-pyrazoles (EPPs) as corrosion inhibitors	81
3.2. 2, 6diaminopyridine as corrosion inhibitors	111
3.3. Imidazole derivatives as corrosion inhibitors	140
3.4. Pyrazolopyridine as corrosion inhibitors	166
CHAPTER 4: SUMMARY	197-203
4.1. Summary	197
4.2. Conclusions	202
4.3. Scope for future work	203
REFERENCES	204-224
LIST OF PUBLICATIONS	225-226