TABLE OF CONTENTS

Page #

Title page I

Holy Quran II

Signature page III

Dedication..... IV

Acknowledgments V

Table of contents VI

Abstract VIII

New accomplishments.....IX

Chapter one : GENERAL BACKGROUND

1-0 Introduction 2

1-1 What is a graph 3

1-2 Definitions of graph..... 4

1-3 Examples of graphs 10

1-4 Operations on graphs 15

1-5 Early history of interplay between Graph Theory and Chemistry 18

Chapter two: MATRIX REPRESENTATION OF MOLECULAR GRAPHS

2-0 Introduction..... 21

2-1 Adjacency matrix 21

Page #

2-2 Incidence matrix..... 27

2-3 Relation between adjacency matrix and incidence matrix..28

2-4 Distance matrix..... 29

2-5 Huckel matrix..... 32

2-6 Eigenvalues and eigenvectors related to physico-chemical Properties of a molecule..... 46

2-7 Evaluation of the eigenvalues and eigenvectors of special matrix 51

Chapter three : ISOMER ENUMERATION

3-0 Introduction..... 64

3-1 Polya enumeration theorem..... 66

Chapter four : TOPOLOGICAL INDICES

4-0 Introduction..... 79

4-1 Wiener index..... 80

4-2 Connectivity index (Randic index)..... 86

4-3 Algebraic connection between topological indices..... 92

4-4 New topological index..... 94

BIBLIOGRAPHY 98