POINT GROUPS OF ORDER AT MOST EIGHT AND THEIR CONJUGACY CLASS GRAPHS

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A dissertation submitted in partial fulfilment of the requirements for the award of the degree of Master of Science

> Faculty of Science Universiti Teknologi Malaysia

> > APRIL 2017

To my beloved mother and father

ACKNOWLEDGEMENT

In The Name of ALLAH, the Most Gracious and the Most Merciful. First and foremost, praise be to Allah s.w.t for giving me His blessing throughout my studies.

I would like to sincerely thank my supervisor, Dr. Fong Wan Heng, for her guidance, encouragement, positive criticisms and support throughout this study. This research would not have been completed and accomplished without her expert advice and unfailing patience.

My sincere thanks go to all lecturers and members of Applied Algebra and Analysis Group (AAAG) UTM who helped in giving me the ideas and motivations in this research. Their views and tips are useful indeed.

I also would like to express my gratitude to my family, especially my parents, who supported me emotionally and financially. Thank you for teaching me to be patient, to be strong and love in what I do. Most importantly, none of this would have been possible without the love and patience of my family. I also would like to express a special word of thanks to my friends for listening, offering me advice, and supporting me throughout this entire process.

Lastly, I would like to thank those involved directly or indirectly in the completion of my research.

ABSTRACT

Point group is a type of group in chemistry, which is a collection of symmetry elements possessed by a shape or form which all pass through one point in space. The stereographic projection is used to visualize the symmetry operations of point groups. On the other hand, group theory is the study about an algebraic structure known as a group in mathematics. This research relates point groups of order at most eight with groups in group theory. In this research, isomorphisms, matrix representations, conjugacy classes and conjugacy class graph of point groups of order at most eight are found. The isomorphism between point groups and groups in group theory are obtained by mapping the elements of the groups and by showing that the isomorphism properties are fulfilled. Then, matrix representations of point groups are found based on the multiplication table. The conjugacy classes and conjugacy class graph of point groups of order at most eight are then obtained. From this research, it is shown that point groups C_1 , C_3 , C_5 and C_7 are isomorphic to the groups Z_1 , Z_3 , Z_5 and Z_7 respectively. Next, point groups $C_{1h} = C_s = C_{1v} = S_1$, $S_2 = C_i$, $C_2 = D_1$ are isomorphic to the group Z_2 , point groups C_4 , S_4 are isomorphic to the group Z_4 , point groups $C_{2h} = D_{1d}, C_{2v} = D_{1h}, D_2$ are isomorphic to the group $Z_2 \times Z_2$, point groups C_{3v} , D_3 are isomorphic to the group S_3 , point groups C_6 , S_6 , $C_{3h} = S_3$ are isomorphic to the group Z_6 . The conjugacy classes of these groups are then applied to graph theory. It is found that the conjugacy class graph for point groups C_{3v} and D_3 are empty graphs; while conjugacy class graph for point groups C_{4v} , D_4 and D_{2d} are complete graphs. As a conclusion, point groups in chemistry can be related with group theory in term of isomorphisms, matrix representations, conjugacy classes and conjugacy class graph.

ABSTRAK

Kumpulan titik ialah sejenis kumpulan dalam kimia yang merupakan koleksi unsur simetri yang dimiliki oleh satu bentuk yang semuanya melalui satu titik dalam ruang. Unjuran stereograf digunakan untuk menggambarkan operasi simetri kumpulan titik. Dari sudut yang lain, teori kumpulan adalah kajian mengenai struktur aljabar yang dikenali sebagai kumpulan dalam matematik. Kajian ini mengaitkan kumpulan titik berperingkat tidak melebihi lapan dengan kumpulan-kumpulan dalam teori kumpulan. Dalam kajian ini, isomorfisma, perwakilan matriks, kelas kekonjugatan dan graf kelas kekonjugatan kumpulan titik berperingkat tidak melebihi lapan telah diperolehi. Isomorfisma antara kumpulan titik dan kumpulan dalam teori kumpulan diperolehi dengan pemetaan unsur-unsur dalam kumpulan dan dengan menunjukkan sifat-sifat isomorfisma dipenuhi. Kemudian, perwakilan matriks bagi kumpulan titik diperolehi berdasarkan kepada jadual pendaraban. Kelas kekonjugatan dan graf kelas kekonjugatan kumpulan titik berperingkat tidak melebihi lapan kemudiannya diperoleh. Dari kajian ini, telah ditunjukkan bahawa kumpulan titik C_1 , C_3 , C_5 dan C_7 berisomorfik dengan kumpulan Z_1, Z_3, Z_5 dan Z_7 masing-masing. Kumpulan titik $C_{1h} = C_s = C_{1v} = S_1$, $S_2 = C_i, \ C_2 = D_1$ berisomorfik dengan kumpulan Z_2 , kumpulan titik $C_4, \ S_4$ berisomorfik dengan kumpulan Z_4 , kumpulan titik $C_{2h} = D_{1d}$, $C_{2v} = D_{1h}$, D_2 berisomorfik dengan kumpulan $Z_2 \times Z_2$, kumpulan titik C_{3v} , D_3 berisomorfik dengan kumpulan S_3 , kumpulan titik C_6 , S_6 , $C_{3h} = S_3$ berisomorfik dengan kumpulan Z_6 . Kelas kekonjugatan kumpulan-kumpulan ini kemudiannya diaplikasikan dalam graf teori. Adalah didapati bahawa graf kelas kekonjugatan bagi kumpulan titik C_{3v} dan D_3 adalah graf kosong; manakala graf kelas kekonjugatan bagi kumpulan titik C_{4v} , D_4 dan D_{2d} adalah graf lengkap. Kesimpulannya, kumpulan titik dalam kimia boleh dikaitkan dengan teori kumpulan dari segi isomorfisma, perwakilan matriks, kelas kekonjugatan dan graf kelas kekonjugatan.

TABLE OF CONTENTS

CHAPTER		TITLE	PAGE		
	DEC	ii			
	DEI	DICATION	iii		
	ACKNOWLEDGEMENT				
	ABS	STRACT	V		
	ABS	STRAK	vi		
	TAF	BLE OF CONTENTS	vii		
	LIS	T OF TABLES	Х		
	LIS	T OF FIGURES	xi		
	LIS	T OF SYMBOLS	xii		
	LIS	T OF APPENDIX	xiv		
1	INT	RODUCTION	1		
	1.1	Introduction	1		
	1.2	Research Background	3		
	1.3	Problem Statements	4		
	1.4	Research Objectives	5		
	1.5	Scope of the Research	5		
	1.6	Significance of the Research	5		
	1.7	Research Framework	6		
	1.8	Dissertation Organization	8		
2	LIT	ERATURE REVIEW	10		
	2.1	Introduction	10		

2.2	Group	Theory	10
	2.2.1	Groups of Order at Most Eight in Group Theory	11
	2.2.2	Conjugacy Classes	12
2.3	Point Operat	Groups in Chemistry and Their Symmetry tions	13
	2.3.1	Identity	15
	2.3.2	Proper Rotation Axis	15
	2.3.3	Planes of Symmetry	17
	2.3.4	Inversion Centre	19
	2.3.5	Improper Rotation Axis	20
2.4	Stereo	graphic Projections	21
2.5	Graph	Theory and Conjugacy Class Graph	22
2.6	Prelim	inaries	24
2.7	Conclusion		
POI	NT GR	OUPS IN CHEMISTRY	29
3.1	Introdu	uction	29
3.2	Symm	etry Operations in Point Groups	29
3.3	Classif	fication of Molecules into Point Groups	35
3.4	Conclu	usion	40
ISO AT N	MORPI MOST I	HISMS OF POINT GROUPS OF ORDER EIGHT WITH GROUPS	42
4.1	Introdu	uction	42
4.2	Isomo	rphism of the Group Z_1 with the Point Group C_1	44
4.3	Isomore C_{1h}, S_2	rphism of the Group Z_2 with the Point Groups T_2 and C_2	45
4.4	Isomo	rphism of the Group Z_3 with the Point Group C_3	49
4.5	Group	s of Order 4	50
	4.5.1	Isomorphism of the Group Z_4 with the Point Groups C_4 and S_4	50
	4.5.2	Isomorphism of the Group $Z_2 \times Z_2$ with the Point Groups C_{2h} , C_{2v} and D_2	54
4.6	Isomo	rphism of the Group Z_5 with the Point Group C_5	58

3

4

	4.7	Group	s of Order 6	60		
		4.7.1	Isomorphism of the Group Z_6 with the Point Groups C_6 , S_6 and C_{3h}	60		
		4.7.2	Isomorphism of the Group S_3 with the Point Groups D_3 and C_{3v}	66		
	4.8	Isomo	rphism of the Group Z_7 with the Point Group C_7	69		
	4.9	Isomo	rphism of the Groups of Order 8	72		
	4.10	Conclu	asion	72		
5	MAT OF (TRIX R ORDEF	REPRESENTATION OF POINT GROUPS R AT MOST EIGHT	74		
	5.1	Introdu	uction	74		
	5.2	Matrix	Representation of Point Groups	75		
		5.2.1	Point Group of Order 1	76		
		5.2.2	Point Groups of Order 2	77		
		5.2.3	Point Group of Order 3	78		
		5.2.4	Point Groups of Order 4	79		
		5.2.5	Point Group of Order 5	85		
		5.2.6	Point Groups of Order 6	86		
		5.2.7	Point Group of Order 7	97		
		5.2.8	Point Groups of Order 8	99		
	5.3	Conclu	asion	126		
6	THE CLA	CON SS GR	JUGACY CLASSES AND CONJUGACY APH OF POINT GROUPS OF ORDER AT			
	MOST EIGHT					
	6.1	Introdu	uction	127		
	6.2	The Co Most H	onjugacy Classes of Point Groups of Order at Eight	127		
		6.2.1	Point Group of Order 1	128		
		6.2.2	Point Groups of Order 2	128		
		6.2.3	Point Group of Order 3	128		
		6.2.4	Point Groups of Order 4	129		
		6.2.5	Point Group of Order 5	129		

	6.2.6	Point Groups of Order 6	129
	6.2.7	Point Group of Order 7	131
	6.2.8	Point Groups of Order 8	131
6.3	The C Order	Conjugacy Class Graph of Point Groups of at Most Eight	136
	6.3.1	Point Groups of Order 6	136
	6.3.2	Point Groups of Order 8	137
6.4	Conclu	usion	139
7 CON	NCLUS	ION	140
7.1	Summ	ary of the Research	140
7.2	Sugge	stions for Further Research	143
DEFEDENCES			145
NEFENCES			143
Appendices A - B			148 - 153

LIST OF TABLES

TABLE NO.	TITLE	PAGE
3.1	The nonaxial groups	30
3.2	The cyclic groups	32
3.3	The axial groups containing mirror planes	34
3.4	The axial groups with multiple rotation axes	35
4.1	Graphical symbols used to represent symmetry elements in stereographic projection	43
4.2	Cayley table of the point group C_1	44
4.3	Cayley table of the point group C_{1h}	46
4.4	Cayley table of the point group S_2	47
4.5	Cayley table of the point group C_2	48
4.6	Cayley table of the point group C_3	49
4.7	Cayley table of the point group C_4	51
4.8	Cayley table of the point group S_4	53
4.9	Cayley table of the point group C_{2h}	54
4.10	Cayley table of the point group C_{2v}	56
4.11	Cayley table of the point group D_2	57
4.12	Cayley table of the point group C_5	59
4.13	Cayley table of the point group C_6	61
4.14	Cayley table of the point group S_6	63
4.15	Cayley table of the point group, $C_{3h} = S_3$	65
4.16	Cayley table of the point group D_3	67
4.17	Cayley table of the point group C_{3v}	68
4.18	Cayley table of the point group C_7	71
4.19	Isomorphism between groups and point groups	73
5.1	Matrix representation for the point groups of order two	78
5.2	Matrix representation for the point groups C_4 and S_4	81

5.3	Matrix representation for the point groups C_{2h} , C_{2v} and D_2	84
5.4	Matrix representation for the point groups C_6 , S_6 and $C_{3h} = S_3$	91
5.5	Matrix representation for the point groups C_{3v} and D_3	96
5.6	Cayley table of the point group C_8	99
5.7	Cayley table of the point group S_8	100
5.8	Matrix representation for the point groups C_8 and S_8	106
5.9	Cayley table of the point group C_{4h}	108
5.10	Cayley table of the point group C_{4v}	111
5.11	Cayley table of the point group D_4	112
5.12	Cayley table of the point group D_{2d}	112
5.13	Matrix representation for the point group C_{4v} , D_4 and D_{2d}	121
5.14	Cayley table of the point group D_{2h}	123
6.1	The number of conjugacy classes and the number of elements in the center of point groups of order at most	
	eight	135

LIST OF FIGURES

FIGURE NO.

TITLE

PAGE

The C_3 axis of ammonia with their operations	16
The structure of benzene showing two sets of three C_2 axes	17
Mirror planes of water molecule (a) vertical plane (b) symmetry plane	18
Horizontal plane in boron trifluoride, BF ₃	18
(a) Dihedral plane lying between two C_2 axes (b) Dihedral plane with no horizontal C_2 axes	19
Inversion operation (a) in square planar XeF_4 (b) in planar $C_2H_2CI_2$	19
The S_6 operation in the staggered form of ethane	20
Illustration of the principle of stereographic projection	21
(a) Königsberg Bridge (b) The graph of the Königsberg bridge problem	22
A five stage procedure for the symmetry classification of molecules	37
The structure of H_2O molecule with the two mirror planes	38
The symmetry elements for ammonia, NH_3 : (a) viewed with the principal axis in the plane of the page; (b) viewed along the principal axis with the mirror planes labelled following the text	39
The structure of ethene molecule (C_2H_4) with three mirror planes and three C_2 axes	40
Stereographic projection for the point group C_1	44
Stereographic projection for the point group C_{1h}	45
Stereographic projection for the point group S_2	46
Stereographic projection for the point group C_2	47
	The C_3 axis of ammonia with their operations The structure of benzene showing two sets of three C_2 axes Mirror planes of water molecule (a) vertical plane (b) symmetry plane Horizontal plane in boron trifluoride, BF ₃ (a) Dihedral plane lying between two C_2 axes (b) Dihedral plane with no horizontal C_2 axes Inversion operation (a) in square planar XeF ₄ (b) in planar $C_2H_2CI_2$ The S_6 operation in the staggered form of ethane Illustration of the principle of stereographic projection (a) Königsberg Bridge (b) The graph of the Königsberg bridge problem A five stage procedure for the symmetry classification of molecules The structure of H ₂ O molecule with the two mirror planes The symmetry elements for ammonia, NH ₃ : (a) viewed with the principal axis in the plane of the page; (b) viewed along the principal axis with the mirror planes labelled following the text The structure of ethene molecule (C ₂ H ₄) with three mirror planes and three C_2 axes Stereographic projection for the point group C_1 Stereographic projection for the point group S_2 Stereographic projection for the point group C_2

4.5	Stereographic projection for the point group C_3	49
4.6	Stereographic projection for the point group C_4	51
4.7	Stereographic projection for the point group S_4	52
4.8	Stereographic projection for the point group C_{2h}	54
4.9	Stereographic projection for the point group C_{2v}	55
4.10	Stereographic projection for the point group D_2	57
4.11	Stereographic projection for the point group C_5	59
4.12	Stereographic projection for the point group C_6	61
4.13	Stereographic projection for the point group S_6	62
4.14	Stereographic projection for the point group C_{3h}	64
4.15	Stereographic projection for the point group D_3	66
4.16	Stereographic projection for the point group C_{3v}	68
4.17	Stereographic projection for the point group C_7	70
6.1	Conjugacy class graph of point group C_{3v}	137
6.2	Conjugacy class graph of point group C_{4v} , K_3	138

LIST OF SYMBOLS

*	-	Binary operation
Z_n	-	Cyclic group
K_n	-	Complete graph
cl(a)	-	Conjugacy class of a
point group C_{3v}	-	Cyclic point group with 3 vertical planes
e	-	Element of
≡	-	Equivalent
FC	-	Finite conjugacy
O_h	-	Full octahedral group
T_d	-	Full tetrahedral group
G	-	Group
Γ	-	Graph
gcd(a,b)	-	Greatest common divisor of a and b
I, I_h	-	Icosahedral group
E	-	Identity element
S_n	-	Improper rotation
i	-	Inversion centre
\cong	-	Isomorphism
$C_{\infty v}$	-	Linear point group
$D_{\infty h}$	-	Linear point group
σ	-	Plane of symmetry
C_n	-	Proper rotation
K(G)	-	The number of conjugacy classes in G
T	-	Regular tetrahedron with no planes of reflection
T_h	-	Regular tetrahedron with centre of inversion

D(R)	-	Transformation matrix
0	-	Octahedron
r_E	-	Vector of identity
ϕ	-	Phi
$V(\Gamma)$	-	Vertices of a graph Γ

LIST OF APPENDIX

APPENDIX TITLE

А	Multiplication tables for groups of order 1 to 7	148
В	Conjugacy classes of point groups of order at most 8	152

PAGE

CHAPTER 1

INTRODUCTION

1.1 Introduction

Group theory is the study about an algebraic structure known as group in mathematics and abstract algebra. It is also a mathematical branch in which symmetry of molecules can be determined. Besides being the systematic treatment of symmetry, it is a powerful tool that simplifies the process of obtaining information about molecules. For instance, molecules are classified based on their symmetry properties and after the properties are identified, the molecules are then assigned to their point groups. Both symmetry and group theory provide a formal method for description of the geometry of objects by describing the patterns in their structure. In this research, group theory will be related to the field of chemistry.

There are many applications of symmetry concepts in the different branches of sciences [1]. Symmetry and point groups have been recognized as the essential concepts for chemists. Many of the molecules consist of symmetry; some of the molecules have no symmetry while some are highly symmetrical. Symmetry is very important in the structure and characteristic of molecules. The symmetry properties of molecules can be classified based on their symmetry characteristics. There are only four types of symmetry elements and operations which are considered in treating the symmetry of molecules which are symmetry planes and reflection, the inversion centre, proper axes and proper rotations, improper axes and improper rotations [2].

In chemistry, there is one type of group called a point group. A point group is a collection of symmetry elements possessed by a shape or form in which all pass through one point in space [3]. It consists of all symmetry operations that are possible for every molecule. This means that the number and types of symmetry elements in the molecule constitutes the point group. A molecular group is known as a point group or symmetry group because there exists a point in a molecule that is not affected by any kind of operations of the molecular symmetry group [4]. The notation used to represent point group of a molecule is the Schoenflies notation which is commonly used by spectroscopists and chemists. Crystallographers prefer to use the Hermann-Mauguin system which is applied to both point and space groups [1]. Among all the point groups, this dissertation focuses on point groups of order at most eight.

For each of the point groups, the symmetry operations in a group can be represented by using matrices. The concepts of matrices in algebra are applied to the elements in point groups so that the relation between group theory and chemistry can be seen. In 2013, Thomas *et al.* [5] mentioned that one particular way to describe the symmetry operations of a molecule is by using the term of a transformation matrix, D(R). Then, Bernath [6] in 2015 stated that the simplest way to generate a matrix representation of a group is by considering the effect of a symmetry operation on a point

$$P = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

in space where the point is located in a real three-dimensional space. Besides that, the groups in group theory and certain point groups in chemistry can be mapped by using isomorphism. An isomorphism is a map that preserves sets and relations among elements. Isomorphism between point groups and groups in group theory helps to relate the classes of point groups with graph theory, which is discussed next.

Graph theory has been rapidly moving into the mainstream of mathematics and has an increased demand in the application of mathematics. A graph is a connection between vertices (points) and edges (lines). Real-life situations can be applied into a graph such as biochemistry (genomics), electrical engineering (communications networks and coding theory), computer science (algorithms and computations) and operations research (scheduling). This research will focus on a type of graph called conjugacy class graph. In order to obtain the conjugacy class graph, the concept of conjugacy class is applied. In group theory, conjugacy class is a method of partitioning the elements of a group in which members of the same conjugacy class share many properties. Therefore, the conjugacy class of a group obtained can be used and applied in graph theory. Bertram *et al.* [7] in 1990 introduced a conjugacy class graph where its vertex set is the set of non-central classes of a group. Then, the two distinct vertices are connected by an edge if the greatest common divisor of the size of conjugacy classes is greater than one.

1.2 Research Background

Point group is an important property of molecules that is widely used in some branches of chemistry, which are spectroscopy, quantum chemistry and crystallography. A point group can be used to classify the shapes of molecules based on their symmetry elements. It is known as point groups because all symmetry elements such as points, lines and planes will intersect at a single point. The idea of point groups has been used in vibrational spectroscopy and the molecular orbital description of chemical bonding [8].

On the other hand, group theory is the study of groups and also the study of symmetry since the set of all symmetries of any object form a group. The two basic concepts in group theory needed when performing an operation to a molecule are the symmetry operations and symmetry elements. There are five elements in point groups which are the identity, plane of symmetry, inversion centre, proper rotation axis and improper rotation axis, denoted as E, σ , i, C_n and S_n respectively. Besides, the point groups are found to be isomorphic to certain groups in group theory. In 2004, Fong [9] has determined the isomorphism of groups of order eight with certain point groups. By

obtaining the symmetry operations for each of the point groups, those elements can be represented by a matrix. This is known as matrix representation of point group. In order to categorize all symmetry elements in a point group, another important concept in group theory that can be used is known as a class or a conjugacy class. The concepts of conjugacy class of groups can then be applied in graph theory.

Some researchers studied about the conjugacy class graph of groups in group theory. For instance, Moradipour *et al.* in 2013 studied about certain properties of the conjugacy classes graph which are structured on some metacyclic 2 - groups [10]. They have shown that the chromatic number and clique number of the graph are identical. In the same year, Omer *et al.* in [11] have found the probability that an element of a group fixes a set and focused on the orbit graph and graph related to conjugacy class graph.

1.3 Problem Statements

Point group in chemistry is used to describe the symmetry of molecules and a condensed representation of the symmetry elements a molecule may posses includes both bond and orbital symmetry. The molecular symmetry helps in understanding the molecular structure besides predicting many molecular properties. Moreover, point groups can give rise to a character table, that is the complete set of irreducible representation of point groups. Over the years, many researches have been done on the topic of point groups. The transformation of symmetry elements of point groups is used to obtain the character table. This research will focus on the relation of point groups of order at most eight in chemistry with group theory .

In this research, the isomorphism of point groups of order at most eight in chemistry and groups in group theory is determined. Besides, matrix representation of point groups of order at most eight is also determined. Then, the conjugacy classes of point groups are used to relate with the conjugacy class graph.

1.4 Research Objectives

The objectives of this research are:

- 1. To determine the isomorphisms of point groups of order at most eight with groups.
- 2. To determine the matrix representation of point groups of order at most eight.
- 3. To generate the conjugacy classes of point groups of order at most eight and relate them with the conjugacy class graph.

1.5 Scope of the Research

This research mainly focuses on the point groups of order at most eight. Besides, the conjugacy class graphs of point groups are obtained by applying the concept of conjugacy class in graph theory.

1.6 Significance of the Research

In chemistry, it is important to find the symmetry of molecules since chemists classify molecules based on their symmetry. The basic symmetry elements and operations are essential in determining the symmetry classification which is known as the point group of different molecules. This research relates the symmetry in point groups with group theory in mathematics using the concept of isomorphism. In this dissertation, the symmetry operations of point groups that have been classified are represented using the matrices. Besides, the graph of the conjugacy classes of point group in the classification is found. Thus, the classes of point groups can be related to the conjugacy class graph in order to model the pairwise relation between the classes of point groups.

1.7 Research Framework

This research involves two fields which are group theory and chemistry. It relates groups in group theory with point groups of order at most eight in chemistry. This research is divided into four parts. The first part is about symmetry of molecules, which is significant to researchers in chemistry's field. Here, group theory can be used as a tool to determine symmetries of molecules. The symmetry of molecules is determined based on the symmetry operations performed with respect to symmetry elements. Next, point groups and groups are related by using the concept of isomorphism. The mapping between these two groups must fulfil the properties of isomorphism which are one-toone, onto and operation preserving. The Cayley table of each point groups is determined in order to show the operation preserving.

Then, the concept of matrix is used in the matrix representation of point groups. The symmetry operations in point groups are presented in the set of matrices that reflect the Cayley table. For the last part, conjugacy classes of point groups of order at most eight are determined. The conjugacy classes are then applied in graph theory, a graph known as conjugacy class graph. Lastly, the conjugacy class graph of each of the point groups is determined by finding the greatest common divisor (gcd) of the order of each pair of the conjugacy classes. The research framework is given in Figure 1.1.



Figure 1.1 Research framework

1.8 Dissertation Organization

This dissertation comprises of seven chapters. The first chapter serves as an introduction to the whole dissertation. It mentions the relation of point groups in chemistry with group theory in term of the symmetry concepts. Besides, the concept of isomorphism, matrix representation, conjugacy classes and conjugacy class graph are also presented. In addition, Chapter 1 also includes the research background, problem statements, research objectives, scope of the research, significance of the research and research framework.

Next, in Chapter 2, the literature review of this research is presented. This includes some concepts of groups in group theory, conjugacy classes, point groups in chemistry with their symmetry operations and stereographic projections. Some previous researches on the conjugacy classes, and conjugacy class graph are included too. Moreover, some preliminaries used in this research are also provided in this chapter.

Chapter 3 presents the point groups in chemistry. In this chapter, symmetry operations in point groups are presented. Besides, classification of molecules into point groups are provided. Also, some examples are presented to illustrate how to allocate molecules into their respective point groups.

In Chapter 4, the isomorphisms of point groups of order at most eight with groups are discussed. Here, the mappings between elements in groups and point groups of order at most eight are presented and are shown to be an isomorphism. Also, the Cayley tables of these point groups and their stereographic projections are shown in this chapter.

In Chapter 5, the matrix representation of point groups is introduced. Here, the symmetry operations in each of the point groups are presented by using matrices. These matrix representations are obtained based on the Cayley table of the respective point groups.

The conjugacy classes and conjugacy class graph of point groups of order at most eight are discussed in Chapter 6. By using the definition of conjugacy class, the conjugacy classes of these groups are determined. Then, using the conjugacy classes, the conjugacy class graphs are then found using their definition.

Lastly, Chapter 7 presents the summary of this research. Some suggestions for future research are also given in this chapter.

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