SOME CHARACTERIZATIONS OF GROUPS OF ORDER 8

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To my beloved father, mother and sister

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ABSTRACT

Group theory is a branch of mathematics which concerns with the study of groups. It has wide applications in other fields too including chemistry. This research focuses on groups of order 8 and their irreducible representations. There are five groups of order 8, namely D_4, Q, C_8, $C_2 \times C_4$ and $C_2 \times C_2 \times C_2$. For any group, the number of possible representative sets of matrices is infinite, but they can all be reduced to a single fundamental set, called the irreducible representations of the group. Burnside method and Great Orthogonality Theorem method are both used to obtain irreducible representations of all groups of order 8. Then, comparisons of both methods are made. Irreducible representation is actually the nucleus of a character table and is of great importance in chemistry. Groups of order 8 are isomorphic to certain point groups. Point groups are symmetry groups which leave at least one point in space fixed under all operations. In this research, isomorphisms from four out of five groups of order 8, namely D_4, C_8, $C_2 \times C_4$ and $C_2 \times C_2 \times C_2$, and isomorphisms from proper subgroups of Q to certain point groups are determined.

TABLE OF CONTENTS

CHAPTER	TITLE	PAGE
1	INTRODUCTION	1
	1.1 Introduction	1
	1.2 Objectives	4
	1.3 Scope of Study	4
	1.4 Introduction to Each Chapter	4
2	SOME BASIC CONCEPTS	6
	2.1 Introduction	6
	2.2 Some Basic Definitions	6
	2.3 Groups of Order 8	11
	2.3.1 Non-Abelian Groups of Order 8	11
	2.3.2 Abelian Groups of Order 8	12
	2.4 Reducible and Irreducible Representations	12
	2.5 Symmetry Operations	13
	2.6 Stereographic Projection	14
	2.7 Conclusion	15

3 IRREDUCIBLE REPRESENTATIONS OF GROUPS OF ORDER 8 USING BURNSIDE METHOD 17

3.1 Introduction 17
3.2 Burnside Method 18
3.3 Irreducible Representations of Dihedral Group, D_4 19
3.4 Irreducible Representations of Quaternion Group, Q 23
3.5 Irreducible Representations of Cyclic Group of Order 8, C_8 24
3.6 Irreducible Representations of $C_2 \times C_4$ 28
3.7 Irreducible Representations of $C_2 \times C_2 \times C_2$ 32
3.8 Conclusion 36

4 IRREDUCIBLE REPRESENTATIONS OF GROUPS OF ORDER 8 USING GREAT ORTHOGONALITY THEOREM METHOD 38

4.1 Introduction 38
4.2 Great Orthogonality Theorem Method 39
4.3 Irreducible Representations of Dihedral Group, D_4 41
4.4 Irreducible Representations of Quaternion Group, Q 42
4.5 Irreducible Representations of Cyclic Group of Order 8, C_8 43
4.6 Irreducible Representations of $C_2 \times C_4$ 45
4.7 Irreducible Representations of $C_2 \times C_2 \times C_2$ 47
4.8 Comparisons of The Two Methods 48
4.9 Conclusion 50

5 ISOMORPHISMS OF GROUPS OF ORDER 8 WITH CERTAIN POINT GROUPS 51

5.1 Introduction 51
5.2 Isomorphisms of D_4 52
5.2.1 D_4 Isomorphic to Point Group D_4 53

5.2.2 D_4 Isomorphic to Point Group C_{4v} 54
5.2.3 D_4 Isomorphic to Point Group D_{2d} 56
5.3 Isomorphisms of C_8 58
5.3.1 C_8 Isomorphic to Point Group C_8 58
5.3.2 C_8 Isomorphic to Point Group S_8 59
5.4 $C_2 \times C_4$ Isomorphic to Point Group C_{4h} 61
5.5 $C_2 \times C_2 \times C_2$ Isomorphic to Point Group D_{2h} 63
5.6 Isomorphisms of Subgroups of Q 65
5.6.1 Subgroup of Order 1 66
5.6.2 Subgroup of Order 2 66
5.6.3 Subgroups of Order 4 68
5.7 Conclusion 71

6 SUMMARY 72

6.1 Conclusion 72
6.2 Suggestions 76

REFERENCES 77

Appendices A-C 79-89

LIST OF TABLES

TABLE NO.	TITLE	PAGE
3.1	Classes in D_4 and their elements	20
3.2	Multiplication table of C_4 times C_4	20
3.3	Characters of the irreducible representations of D_4 in terms of d_k	22
3.4	Irreducible representations of D_4	23
3.5	Classes in Q and their elements	23
3.6	Irreducible representations of Q	24
3.7	Classes in C_8 and their elements	24
3.8	Characters of the irreducible representations of C_8 in terms of d_k	27
3.9	Irreducible representations of C_8	28
3.10	Classes in $C_2 \times C_4$ and their elements	29
3.11	Characters of the irreducible representations of $C_2 \times C_4$ in terms of d_k	30
3.12	Irreducible representations of $C_2 \times C_4$	32
3.13	Classes in $C_2 \times C_2 \times C_2$ and their elements	32
3.14	Characters of the irreducible representations of $C_2 \times C_2 \times C_2$ in terms of d_k	34
3.15	Irreducible representations of $C_2 \times C_2 \times C_2$	36
4.1	Table where the elements inside are obtained by group multiplication	44
4.2	Table after reducing the powers of ϵ's to modulo 8	45

LIST OF FIGURES

FIGURE NO.	TITLE	PAGE
2.1	Stereographic Projection	15
5.1	Point Group D_4	53
5.2	Point Group C_{4v}	54
5.3	Point Group D_{2d}	56
5.4	Point Group C_8	58
5.5	Point Group S_8	60
5.6	Point Group C_{4h}	62
5.7	Point Group D_{2h}	63
5.8	Point Group C_1	66
5.9	Point Group C_{1h}	67
5.10	Point Group C_2	67
5.11	Point Group S_2	68
5.12	Point Group C_4	69
5.13	Point Group S_4	70

LIST OF SYMBOLS

1	-	identity element in a group
a^b	-	$b^{-1}ab$, conjugation of a by b
$c_{ij,s}$	-	class multiplication coefficient
C_n	-	Cyclic group of order n
$G \times H$	-	direct product of groups G and H
d_k	-	dimension of the kth irreducible representation
D_4	-	Dihedral group
E	-	identity element in point group
G	-	Group
h	-	order of a class
l_i	-	dimension of the ith irreducible representation
point group C_n	-	Cyclic point group
point group C_{nh}	-	Cyclic point group with horizontal planes
point group C_{nv}	-	Cyclic point group with vertical planes
point group D_n	-	Dihedral point group
point group D_{nd}	-	Dihedral point group with planes between axes
point group D_{nh}	-	Dihedral point group with horizontal planes
point group S_n	-	point group with improper rotations
Q	-	Quaternion group
R	-	operation in a group
Γ_i	-	ith irreducible representation
δ_{jk}	-	Kronecker delta

ϕ - an isomorphism

$\chi_i{}^j$ - character of elements in class C_i in the irreducible representation labelled by j

$\chi_i(R)$ - character of the irreducible representation of R in the ith irreducible representation

$\cong$ - isomorphic

LIST OF APPENDICES

APPENDIX	TITLE	PAGE
A	Multiplication table for groups of order 8	79
B	Multiplication table for point groups of order 1, 2, 4 and 8	82
C	Multiplication table for subgroups of Q	88

CHAPTER 1

INTRODUCTION

1.1 Introduction

Group theory is a branch of mathematics which concerns with the study of groups. It is also the study of symmetry since the collection of symmetries of some object preserving some of its structure forms a group. An important class of groups is the set of permutation groups, where the elements are permutations of some set, and the group operation is composition. A second large class of groups is the linear groups. Furthermore, another important class of groups is the set of Abelian groups, those whose elements commute. There are internal features which can be examined in group theory, for instance, subgroups, abelianization, subgroup lattice and mapping between groups. With all these unique features, group theory can be used in various fields, for example, in physics, chemistry and biology.

This research discusses the irreducible representations of all groups of order 8. Individual atoms, bonds, atomic orbitals and any other piece of an overall molecule respond to symmetry operations in different ways. There is a classification system associated with each point group to classify the behavior of a molecule. A set of irreducible representations represents the ways a particular bond, atom or sets of atoms may respond to a given set of symmetry operations. Irreducible representation is actually the nucleus of the character table of a group. A character table is a table where the characters of each of the classes are tabulated. Obtaining the irreducible representations associated with a given bond, atoms or sets of atoms is a convenient way of labelling orbitals for reference. Besides, irreducible representations determines which sets of atomic orbitals can combine with each other to form molecular orbitals. Lastly, an irreducible representation of a molecule determines the number and nature of vibrational motions for the molecule by removing the irreducible representations that correspond to the translation and rotation of the molecule.

In this dissertation, two methods to obtain the irreducible representations of a group are discussed, namely Burnside method and Great Orthogonality Theorem method. For Burnside method, three formulas are used to obtain the class multiplication coefficients, characters of the irreducible representations in terms of d_k, where d_k is the dimension of the kth irreducible representation, and the numerical values for d_k. Great Orthogonality Theorem method mainly uses the Great Orthogonality Theorem and five important rules. However, for different types of groups, for instance, cyclic groups and direct product groups, a little different approach is needed when Great Orthogonality Theorem method is used. Both methods are then discussed for their efficiency.

For this dissertation, only all groups of order 8 are discussed. There are five groups of order 8 which consist of two non-Abelian groups and three Abelian groups. The groups are all written in group presentation form, that is the form of a group with a set of generators and certain relations for the generators to satisfy.

The first non-Abelian group of order 8 is the dihedral group, D_4, with group presentation $\langle a, b | a^4 = b^2 = 1, a^b = a^{-1} \rangle$. The second non-Abelian group of order 8 is the quaternion group, Q, with group presentation $\langle a, b | a^4 = 1, b^2 = a^2, a^b = a^{-1} \rangle$.

The first Abelian group of order 8 is the cyclic group, C_8, with group presentation $\langle a|a^8 = 1\rangle$. The second Abelian group of order 8 is the direct product of the groups C_2 with C_4, which is $C_2 \times C_4$, with group presentation $\langle a,b|a^2 = b^4 = 1, ab = ba\rangle$. The third Abelian group of order 8 is the direct product of three copies of C_2, which is $C_2 \times C_2 \times C_2$, with group presentation $\langle a,b,c|a^2 = b^2 = c^2, ab = ba, ac = ca, bc = cb\rangle$.

Next, the relation between groups of order 8 with various point groups is found.

In chemistry, there are various point groups. Point groups are symmetry groups which leave at least one point in space fixed under all operations [1]. Among all point groups, those of order 8 are point groups D_4, C_{4v}, D_{2d}, C_8, S_8, C_{4h} and D_{2h}.

Mappings, called isomorphisms, are found between groups of order 8 and certain point groups. Isomorphism is also known as mathematical equivalence between two or more groups. Isomorphic groups possess the same structure in the character table, but differ in symmetry operations.

Practical importance of isomorphism is in reducing to a minimum the number of groups that need to be studied. As for theoretical importance, it is to emphasize the fact that group theory is concerned with the structure of its multiplication table, since if two groups are isomorphic, there is some way of re-labeling the elements so that the multiplication table becomes identical despite the difference in elements of the groups [2].

In order to visualize the symmetry operations in groups, stereographic projection is used. Stereographic projection is a way of mapping points on the surface of a sphere onto a two-dimensional figure. It can be used to represent a symmetry operation in three dimensions because both a starting point and any points generated from it by a symmetry operation can be shown on a two-dimensional figure.

1.2 Objectives

The objectives of this research are

(i) to obtain the irreducible representations of all groups of order 8 using Burnside method and Great Orthogonality Theorem method,

(ii) to make comparisons of the two methods in obtaining the irreducible representations,

(iii) to find the isomorphisms of all groups of order 8 (except the quaternion) with certain point groups,

(iv) to find the isomorphisms of the proper subgroups of quaternion group of order 8, Q, with certain point groups.

1.3 Scope of Study

This report mainly focuses on obtaining the irreducible representations of all groups of order 8 using Burnside method and Great Orthogonality Theorem method. Besides, isomorphisms of all groups of order 8 with certain point groups are determined. In the case where a particular group is not isomorphic to any point group, isomorphism of its proper subgroups with certain point groups are discussed.

1.4 Introduction to Each Chapter

Chapter 1 is the introduction chapter which gives the general idea of the whole research. It states the objectives and scope of study. Besides, introduction to each chapter are mentioned.

Chapter 2 introduces some basic definitions and concepts related to this research. Some definitions discussed are group, subgroup, order of a group, order of an element, Abelian group, cyclic group, point group, class and isomorphism. Besides, all groups of order 8, reducible and irreducible representations and multiplication table are mentioned. Moreover, some concepts in chemistry are also included, among them are symmetry operations and character table.

Chapter 3 describes Burnside method to obtain the irreducible representations of all groups of order 8. In this method, three formulas are used to obtain the class multiplication coefficients, characters of the irreducible representation in terms of d_k, where d_k is the dimension of the kth irreducible representation, and the numerical values for d_k. Then, the advantages and disadvantages of this method are discussed.

Next, Great Orthogonality Theorem method is used to obtain the irreducible representations of all groups of order 8 in Chapter 4. This method mainly uses the Great Orthogonality Theorem and five important rules. But for groups such as cyclic groups and direct product groups, there are specific rules to be followed. Lastly, the advantages and disadvantages of this method are also discussed.

In Chapter 5, isomorphisms of all groups of order 8 with certain point groups are obtained. The point groups mentioned are D_4, C_{4v}, D_{2d}, C_8, S_8, C_{4h} and D_{2h}. In the case of the quaternion group of order 8, Q, where there is no point group isomorphic to it, isomorphism of its proper subgroups with certain point groups are discussed. In order to visualize the order of each symmetry operation for the point groups, stereographic projection is used. Using this projection, points on the surface of a sphere can be mapped onto a two-dimensional figure.

Finally, Chapter 6 is the summary for this report. It summarizes what have been discussed in the previous chapters and also includes some suggestions for further research that can be done.