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Group Theory in Chemistry

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Contents

CONTENTS **2**
ABSTRACT **3**
ACKNOWLEDGEMENTS **4**
CHAPTER 1: INTRODUCTION **5**
CHAPTER 2: GROUP THEORY IN CHEMISTRY AT WPI **6**
2.1 MA3823: Group Theory 6
2.2 CH3410: Principles of Inorganic Chemistry 10
CHAPTER 3: COLLEGE COURSES IN GROUP THEORY IN CHEMISTRY **12**
3.1 Undergraduate Courses 12
3.1.1 Massachusetts Institute of Technology 12
3.1.2 Stanford University 13
3.1.3 Arizona State University 14
3.1.4 Texas Agricultural and Mechanical 14
3.1.5 University of California-Berkeley 16
3.1.6 Michigan Technological University 16
3.1.7 Princeton University 17
3.1.8 University College London 17
3.1.9 Wayne University 18
3.1.10 Case Western Reserve University 18
CHAPTER 4: LITERATURE ANALYSIS **19**
4.1 Group Theory in Chemistry Texts 19
4.1.1 Chemical Applications of Group Theory 3rd Edition 19
4.1.2 Molecular Aspects of Symmetry 20
4.1.3 Symmetry through the Eyes of a Chemist 21
4.1.4 Group Theory and Symmetry in Chemistry 22
4.1.5 Group Theory in Chemistry and Spectroscopy 23
4.1.6 Molecular Symmetry and Spectroscopy 24
4.1.7 The International Encyclopedia of Physical Chemistry and Chemical Physics 24
4.2 Chemistry in Group Theory Texts 26
CHAPTER 5: CHEMISTRY IN MATHEMATICS **29**
Burnside Rings: Application to Molecules of Icosahedral Symmetry 29
CHAPTER 6: MATHEMATICS IN CHEMISTRY **46**
Group Theory and the Near-Ultraviolet Absorption Spectrum of Gas-Phase Benzene 46
BIBLIOGRAPHY **50**

Abstract

This MQP examines the teaching practices concerning group theory in chemistry and chemistry in group theory at WPI as well as other colleges. The influence and importance of the interaction of the two subjects on each other is exemplified by its prevalence in academic texts as well as a recent research article in the mathematical sciences with applications in chemistry and a recent chemistry experiment, whose analysis used group theory as a tool.

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Chapter 1: Introduction

Felix Klein in his Erlangen program in 1872 suggested studying the intrinsic properties of an object by studying the group of transformation that leaves the object unchanged. This basic idea profoundly influenced group theory.

Group theory is part of algebra. In standard undergraduate education in mathematical sciences, group theory is introduced within abstract algebra. In contrast to the calculus sequence, applications are not the main focus of the algebra sequence. Chemistry provides natural applications for group theory in the spirit of Felix Klein, but these are not always taught.

This project looks explicitly for applications of group theory to chemistry. To this end we examine how group theory is taught at WPI and other comparable universities. Moreover, we examine whether or not group theory is found in chemistry courses. What level of mathematics are chemistry majors required to know?

Do there exist new publications in the mathematical sciences with applications of group theory to chemistry? Do chemists use group theory in their work? We can confidently answer yes to both questions after examining the literature.

Chapter 2: Group Theory in Chemistry at WPI

2.1 MA3823: Group Theory

All undergraduate students majoring in mathematical sciences at WPI are required to take either Group Theory (MA3823) or Rings and Fields (MA3825). Both courses are offered once a year alternating years. The entry in the WPI course catalog for Group Theory is the following:

> This course provides an introduction to one of the major areas of modern algebra. Topics covered include: groups, subgroups, permutation groups, normal subgroups, factor groups, homomorphisms, isomorphisms and the fundamental homomorphism theorem. (WPI Mathematical Sciences Department Course Catalog 2007-2008)

I took Group Theory in fall of 2006 with a visiting professor named Jason Williford. The primary text was *Contemporary Abstract Algebra* (Gallian, 2004) by Joseph A. Gallian. According to the course syllabus:

> The aim of this course is to introduce students to some of the basic concepts and techniques of abstract algebra. This will be achieved through a study of an algebraic structure called a group, an algebraic object with one associative operation that satisfies certain properties…The symmetries of a mathematical object also form a group; for this reason group theory can be thought of as a study of symmetry from an algebraic perspective. (WPI Mathematical Sciences Department Course Catalog 2007-2008)

The major topics covered were:

- Functions
- Finite Groups and Subgroups
- Modular Arithmetic
- Subgroup Tests
- Cyclic Subgroups
- Center of a Group
- Cyclic Groups
- Group Generators
- Equivalence Relations
- Permutations and Transpositions
- Isomorphisms
- Automorphisms
- Homomorphisms
- Innermorphisms
- Group Stabilizers
- Orbit Theory
- External and Internal Direct Products
- Normal Subgroups
- Factor Groups

An introductory concept of the course was to classify the symmetries of a square. A square is an object which is simple to describe and manipulate. We can easily imagine it as an ideal physical structure with its points, edges and faces marked and colored, so that we can keep track of rotations, which are orientation preserving transformations, and reflections, which are orientation reversing transformations. We see that studying a geometric object as simple as a square, we get to comprehend quite a few abstract concepts. The dihedral group can be defined as the group of symmetries of a regular n-gon, and such a geometric definition is easier to grasp because it is a very visual as opposed to an abstract definition. We learned that the dihedral group (D_n) was defined as $D_n = \{e, r^k, s, r^k s\}$ (k and n both integers) where:

- The *identity operation* (e) causes no change
- The *rotation operation* (r^k) (also called *proper rotation*) where
  $k = \{1, n\}$ is a counterclockwise rotation of k ($360^o/n$) about a rotation axis.
  When $k = n$, $r^n = e$ (since a rotation of 360^o is the identity operation)
- The *reflection operation* (s) exchanges left and right, as if each point had moved perpendicularly through the plane to a position exactly as far from the plane as when it started. If k is even, ($k = 2p$) $s^{2p} = e$.
- A *rotation-reflection operation* ($r^k s$) (sometimes called an *improper rotation*) requires a rotation of k ($360^o/n$) followed by reflection through a plane perpendicular to the axis of rotation.

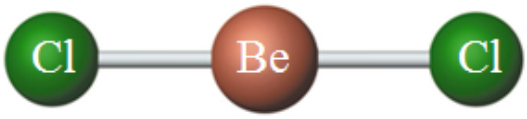
At the end of the term we had the option to turn in a research paper, worth 10% of our grade, which looked at applications of group theory to other areas such as representation theory, character theory, chemistry, physics, classification theorem, coding theory, and matrix groups.

For my research paper, I chose to look at applications of group theory to chemistry because of my strong chemistry background.

Motivated by my experiences in chemistry, the first connection to group theory that came to my mind was the concept of symmetry groups and symmetry operations. If there was group theory representation for regular polygons, could there also be for atoms and molecules? After some preliminary research looking into specific applications of group theory to chemistry I decided to look primarily at symmetry operations of simple linear molecules from both a geometric and group theoretical approach. I chose a basic linear molecule Beryllium Chloride ($BeCl_2$) which has the following molecular representations:



(1)



(2)

Observing figure (1), the Lewis structure of $BeCl_2$, each chlorine atom has seven valence electrons and the central beryllium atom has two valence electrons. As such, beryllium forms a single polar covalent bond with each chlorine atom. Looking at the two ends of the molecule, it is easy to see that each chlorine atom has three pairs of valence electrons that are not in bonds. Since electrons all carry the same negative (-) charge, it is inherent in their nature to repel each other. As such, the chlorine atoms will be the optimal distance apart that the molecule allows. In this case, to maximize distance, the atoms form a 180º angle with the centralized atom as a vertex. Looking at figure (2) it is very easy to see the symmetry operations for $BeCl_2$:

(*i*) a rotation around a central horizontal C_∞ axis
(*ii.)* a reflection about a central and then
(*iii.)* a composition of (*i.*) and (*ii.*) or a rotation followed by a reflection.
The identity operation (*e*) is also a symmetry operation.

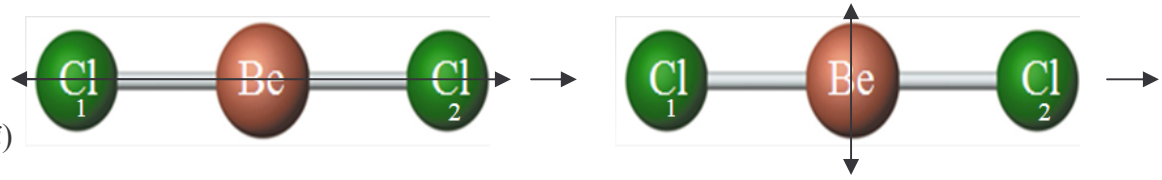
(*i*)



(*ii*)



(*iii*)





2.2 CH3410: Principles of Inorganic Chemistry

At WPI there is only one chemistry course that looks at applications of group theory. *Principles of Inorganic Chemistry* (CH3410) is offered every year and is required for undergraduate chemistry, chemical engineering, and biochemistry majors. There are no stated prerequisites to take the course however it is very unlikely that anyone outside of the three departments would take it. It only assumes you have taken introductory and transition courses in chemistry as you would have to in these disciplines. The course description, as presented in the course catalog, is the following:

> This course provides the fundamental understanding of atomic, molecular and solid state structures and properties. Orbital structures of atoms, symmetry of molecules and point groups are used to understand chemical bonding and reactions. Various acid-base concepts are explored to analyze the acidity of cations and basicity of anions, solubility and precipitations of inorganic compounds, and metal-ligand binding affinities. Redox properties are discussed using Pourbaix diagrams. Thermodynamic stabilities of inorganic species are discussed using acid-base and redox concepts and thermochemical analyses are used to analyze chemical reactivity at atomic, molecular, and solid state level. (WPI Chemistry and Biochemistry Department Coure Catalog 2007-2008)

The current text used is Inorganic Chemistry 3rd Edition (Miessler, 2003) by Gary L. Miessler and Donald A. Tarr. The fourth chapter is titled *Symmetry and Group Theory* and is 36 pages long. The first section of the chapter looks specifically at symmetry elements and operations. The group theory material from this chapter is very introductory and does not require an advanced knowledge of either field but just a basic knowledge of geometry. It states that: "Molecules or any other objects may contain *symmetry elements* such as mirror planes, axes of rotation, and inversion centers. The actual reflection, rotation, or inversion is called the *symmetry operation*…" If a symmetry operation yields a molecule that can be distinguished from the original in any way, then that operation is *not* a symmetry operation of the molecule."

(Miessler, 2003) This text defines the symmetry operations just as any regular group theory textbook would.

The second section of this chapter is where the application of group theory is first mentioned: “Each molecule has a set of symmetry operations that describes the molecule’s overall symmetry. This set of symmetry operation is called the *point group* of the molecule. *Group Theory*, the mathematical treatment of the properties of groups, can be used to determine the molecular orbitals, vibrations, and other properties of the molecule.” (Miessler, 2003) The rest of the section is devoted to showing different examples of point groups and how to classify molecules based on their degrees of symmetry.

The more relevant application of group theory is in the third section titled *Properties and Representations of Groups*. In addition to basic group theory definitions, the section goes on to give detailed definitions and examples of the following components of group theory: matrix representations of symmetry operations, reducible and irreducible representations, character tables, and transformation matrices. All of these components each have their own specific chemical examples and applications. The final section of the chapter goes on to mention these applications and examples.

This chapter does not go into great detail about group theory, since this is a chemistry textbook; however it mentions all the relevant applications of group theory to chemistry. When defining specific elements of group theory the text provides thorough and accurate mathematical definitions while also emphasizing their chemical applications. Overall, chemistry oriented students taking inorganic chemistry using this specific textbook will have a fairly basic and easy introduction to group theory regardless of their math background.

Chapter 3: College Courses in Group Theory in Chemistry

There are several prominent engineering universities, both nationwide and abroad, that have classes dedicated to presenting and teaching applications of group theory to chemistry. These courses are both at the undergraduate and graduate levels. At nearly all the said universities, the courses were chemistry courses that were in the more advanced stages of a degree in chemistry or chemical engineering. Therefore these courses had many prerequisite chemistry courses. However not many of these courses had any real semblance of a math prerequisite which would suggest that the group theory concepts are taught as not only applications, but a very elementary introduction as well.

3.1 Undergraduate Courses

3.1.1 **Massachusetts Institute of Technology** (MIT), Cambridge, Massachusetts

At MIT, the top ranked engineering universities in the country, all undergraduate chemistry students can take 5.04: *Principles of Inorganic Chemistry II*. This class requires that the student has taken the previous course *Principles of Inorganic Chemistry I, Organic Chemistry I, as well as Principles of Chemical Science*. However, despite these prerequisites, this course is classified as a transition course. This course, taught as recently as the fall of 2007, is described by the professor as a:

> Systematic presentation of the chemical applications of group theory. Emphasis on the formal development of the subject and its applications to the physical methods of inorganic chemical compounds. Against the backdrop of electronic structure, the electronic, vibrational, and magnetic properties of transition metal complexes are presented and their investigation by the appropriate spectroscopy described. (Massachusetts Institute of Technology Chemistry Department Course Catalog 2007-2008)

Specifically, the course syllabus presents the following group theory concepts:

- Symmetry elements and operations
- Operator properties and mathematical groups
- Similarity transforms , classes and representations
- Characters and character tables
- Molecular point groups

After these concepts are presented, the course diverges into more chemistry specific material looking into the chemical applications of the previous material covered.

3.1.2 **Stanford University**, Stanford, California

At Stanford, another of the top ranked engineering school in the nation, undergraduate chemistry students are required to take CHEM 153: *Inorganic Chemistry II.* This course is described in the course catalog as:

> The theoretical aspects of inorganic chemistry. Group theory; many-electron atomic theory; molecular orbital theory emphasizing general concepts and group theory; ligand field theory; application of physical methods to predict the geometry, magnetism, and electronic spectra of transition metal complexes. (Stanford Bulletin: Chemistry Department 2007-2008)

Students desiring to take this course are required to have CHEM 151: *Inorganic Chemistry I* as well as CHEM 171: *Physical Chemistry*. The latter doesn't mention group theory as one of the course components however it is interesting to note that this class has a mathematics prerequisite specifically MATH 51: *Multivariable Calculus*. Although this is not group theory, this was the first chemistry course with a math prerequisite.

3.1.3 **Arizona State University**, Mesa, Arizona

At Arizona State's polytechnic campus, undergraduate chemistry students are required to take CHM545: *Quantum Chemistry I* in which the second major topic covered is "Group Theory for Chemistry." (CHM 545 Quantum Chemistry) This topic specifically looks at the following mathematical components: basics of linear algebra, symmetry operations and modules, point groups, matrix representation of symmetry operations, and finally characters and character tables. The required texts for this class are appropriately both advanced chemistry texts: Symmetry and Spectroscopy (Bertolucci, 1989) by Daniel Harris and Michael D. Bertolucci as well as Quantum Mechanics in Chemistry (Schatz, 2002) by George C. Schatz and Mark A. Ratner. Neither of these texts have very explicit sections on group theory. Nonetheless, the professor's willingness to deviate from the text to introduce specific group theory concepts shows its importance to the course and the subject as a whole.

3.1.4 **Texas Agricultural and Mechanical** (Texas A&M), College Station, Texas

At Texas A&M chemistry students can take Chemistry 673: *Symmetry and Group Theory in Chemistry*. This advanced chemistry course had the following course description:

> The course will provide an introduction to the fundamentals and applications of the theory of group representation in chemistry. After an introduction to the abstract theory of groups is given, applications of symmetry groups will constitute the major emphasis of the course. The student will be encouraged to develop both the formal skills of using group theory to "grind out answers" and to acquire some intuitive and pictorial sense of "what it all means"… (Chemistry 673 Symmetry and Group Theory in Chemistry)

The main text uses is F.A. Cotton's Chemical Applications of Group Theory (Cotton, 1990) and the course is broken down in the following manner:

I. Basic Properties of Groups and Symmetry Groups ~ 2 weeks
- Multiplication of elements closure
- existence of an identity element and reciprocal

- associative law
- noncommutation of operations
- multiplication tables
- subgroups and supergroups
- Symmetry groups
    - symmetry elements and operations
    - assigning point groups (flow chart)
    - examples of subgroups
    - abelian groups, cyclic groups
    - translation groups and crystals — introduction to k-space
- Similarity transformations and classes
    - similarity transformations
    - geometrical significance of classes of symmetry operators

II. Group Representations and Physical Implications ~ 3-4 weeks

- Matrices as representations for symmetry operations
- review of vector and matrix properties; matrix operations
- some special properties of matrices
- character (trace) of a matrix
- orthogonal matrices, matrices as geometric transformation operators
- inverses
- Group representations
- reducible and irreducible representations
- the "Great Orthogonality Theorem" and its consequences
- character tables
- cyclic groups
- translation groups (just special cyclic groups)
- Group theory as a tool in quantum mechanics
- operators in quantum mechanics
- the importance of operators that commute with the Hamiltonian
- symmetry operators as special cases of commuting operators
- the direct product and its uses
- bases for group representations and nonzero matrix elements
- transition probabilities - symmetry aspects
- Symmetry-Adapted Linear Combinations (SALCs) and Bases for Irreducible
- Representations.
- projection operators - "complete" and "incomplete"
- projection operators in the construction of SALCs
- symmetry patterns, SALCs, and the intuitive nature of bases for irreducible
- representations - a pictorial survey (Chemistry 673 Symmetry and Group Theory in Chemistry)

The reason for this particular class structure is mainly due to the text however the class also looks at selected applications of group theory including: Molecular Oribtal Theory, Band

Theory, and Vibration Spectra for six to seven weeks which uses ideas and concepts from a second text, the aforementioned *Symmetry and Spectroscopy*. As the course title suggests, this course is dedicated to investigating and understanding chemical applications of group theory.

3.1.5 **University of California-Berkeley**, Berkeley, California

At UC-Berkeley, another highly ranked engineering school, chemistry students can enroll in Chemistry 104A: *Inorganic Chemistry*. According to the professor:

> "This course is intended primarily as an introduction to inorganic chemistry for undergraduate students. Topics covered will include: atomic structures, periodic trends, symmetry and group theory, inorganic solids, molecular orbital theory, molecular structure, acid-base chemistry, and band theory." (Chemistry 104A, 2007)

Although inorganic chemistry is a relatively advanced course, this particular course appears much earlier in the course sequence that at other schools. Although symmetry and group theory is only one of many elements of this course, the text is titled Molecular Symmetry and Group Theory (Carter, 1998).

3.1.6 **Michigan Technological University**, Houghton, Michigan

At Michigan Tech, undergraduate chemistry students nearing the end of their degree or graduate students can take Chemistry 5540: *Applications of Group Theory in Chemistry*. This course has the following course description: "The predicted power of group theory in chemistry is developed through theory and detailed applications. Emphasizes group theoretical applications to molecular orbital theory, orbital symmetry, ligand field theory, and vibrational spectroscopy." (Michigan Tech Graduate Course Descriptions 2007)

3.1.7 **Princeton University**, Princeton, New Jersey

At Princeton, undergraduate chemistry students can take Chemistry 505: *Group Theory in Chemistry*. This course uses Symmetry through the Eyes of a Chemist (Hagittai, 1986) by István and Magdolna Hargittai as the primary text. This book is very chemistry oriented and does not dedicate a lot to group theory concepts. As such, the course also includes much more supplemental reading material including Cotton's *Chemical Applications of Group Theory*. The course description includes the following components of chemical applications of group theory:

- Examples of symmetry groups: point groups for molecular symmetry, permutation groups for counting isomers and constructing wave functions, rotation groups and angular momenta
- Classification of rigid molecules into point groups. Distinguishing isomers, geometrical and stereo-isomers.
- Principles of Group Theory:
    - matrix representations of groups; subgroup structure and faithful representations;
    - character tables, projection operators, Orthogonality theorem, direct products
    - many particle wave functions (Chemistry 505: Group Theory in Chemistry)

3.1.8 **University College London**, London, England

Finally, looking overseas at University College London, undergraduate chemistry students can take Chemistry 2102: Principles of Inorganic Chemistry. This class uses Inorganic Chemistry (Shriver, 2006) by Duward Shriver and Peter Atkins as well as Concepts and Models of Inorganic Chemistry (Douglas, 1994) by Bodie Douglas, Darl McDaniel, and John Alexander. The course is divided up into four main components the first of these being dedicated to an "Introduction to the Principles and Applications of Group Theory." (UCL Chemistry) This section is broken down in the following way:

Part 1: Revision of Symmetry Operations, Symmetry Elements and Point Groups

Part 2: Group Theory: Some Definitions

- Definition of a group; rules that must be satisfied by the elements of a group.
- Group multiplication tables
- Abelian and non-Abelian groups
- Matrix representations of groups, including matrix multiplication
- Characters of matrix representations
- Irreducible representations
- Reduction of representations; direct sums
- Character tables

Part 3: Group Theory and Chemical Bonding

- Construction of a qualitative molecular orbital energy level diagram for water, including use of the reducing formula and the projection operator for the construction of Symmetry Adapted Linear Combinations (SALCs)
- Construction of qualitative molecular orbital energy level diagrams for ammonia and MH6. (UCL Chemistry)

3.1.9 **Wayne University**, Detroit, Michigan

At Wayne University, graduate students pursuing a master's degree in chemistry can enroll in Chemistry 6040: *Chemical Applications of Group Theory*. This graduate course is described as: "Symmetry in chemical systems, development and use of character tables and applications of group theory to structure, bonding, spectroscopy and reactions." (Chemistry Courses (CHM)) Since the class is at the graduate level, there are more than a few prerequisite chemistry classes. No text is specifically mentioned in the course outline.

3.1.10 **Case Western Reserve University**, Cleveland, Ohio

Another graduate course offered can be found at Case Western Reserve University where graduate chemistry students can take Chemistry 415: *Chemical Applications of Group Theory*. This course is described as "Experimental and semi-empirical treatments of the structures and bonding in chemical systems, based on presentation of symmetry relationships and the theory of point and space groups." (Graduate Chemistry Courses) No specific text is mentioned in the course outline.

Chapter 4: Literature Analysis

4.1 Group Theory in Chemistry Texts

To gain a better understanding of how group theory is presented in college chemistry courses it would be the most logical to look at the primary text books used. Looking at many different texts would reveal a wide spectrum of how different authors in academia present advanced math concepts, specifically group theory and abstract algebra, to chemistry students and conversely. Also, common elements of different texts can help to highlight and understand which specific concepts are most critical to the subject.

4.1.1 Chemical Applications of Group Theory 3rd Edition (Cotton, 1990)

F. Albert Cotton, Texas A&M University, College Station, TX

Frank Albert Cotton was an award winning researcher and a distinguished member of the chemistry community. He was the author of over 1700 articles and in addition this text has been credited with "…introducing generations of chemists to the group theoretical analysis of bonding and spectroscopy." (F. Albert Cotton) According to the preface:

> This book is the outgrowth of a one-semester course which has been taught for several years at the Massachusetts Institute of Technology to seniors and graduate students in chemistry. The treatment of the subject matter is unpretentious in that I have not hesitated to be mathematically unsophisticated, occasionally unrigorous, or somewhat prolix, where I felt that this really helps to make the subject more meaningful and comprehensible for the average student. By the average student, I mean one who does not aspire to be theoretician but who wants to have a feel for the strategy used by theoreticians in treating problems in which symmetry properties are important and to have a working knowledge of the more common and well established techniques. (Cotton, 1990)

Appropriately, his book is the primary text used at both the Massachusetts Institute of Technology (MIT) as well as where he taught, Texas A&M. His admonition in the preface is very interesting because he is admitting that he is "mathematically unsophisticated" and as such implicative that his students will be the same if not more unrefined in mathematics.

From an organizational standpoint, Cotton dedicates many pages to establishing a solid foundation of basic introductory group theory principles to transition to more advanced chemical applications. In total, Cotton offers three chapters (94 pages) dedicated to group theory:

- **Chapter 2: Definitions and Theorems of Group Theory**
  - The defining properties of a group
  - Some examples of groups
  - Subgroups
  - Classes
- **Chapter 3: Molecular Symmetry and the Symmetry Groups**
  - Symmetry elements and operations
  - Symmetry planes and reflections
  - The inversion center
  - Proper axes and proper rotations
  - Improper axes and improper rotations
  - Products of symmetry operations
  - Equivalent symmetry elements
  - General relations among symmetry elements and operations
  - Classes of symmetry operations
- **Chapter 4: Representations of Groups**
  - Representations of groups
  - The "Great Orthogonality Theorem" and its consequences
  - Character tables
  - Representations for cyclic groups

4.1.2 **Molecular Aspects of Symmetry** (Hochstrasser, 1966)

Robin M. Hochstrasser, University of Pennsylvania, Philadelphia, PA

Molecular Aspects of Symmetry is a chemistry text that investigates how mathematical concepts can be applied to help understand different chemical concepts. Specifically:

> The contents of this book have been utilized in two courses given by the author. The first was a one-semester course for seniors at the University of British Columbia; it was clear that good undergraduates were perfectly capable of handling elementary group theory

> and its application to simple quantum chemical problems…The second course was directed at first and second-year graduate students of physical chemistry at the University of Pennsylvania, for which the prerequisites were a previous or current year of quantum chemistry…It has been this author's experience that the study of group theory helps students to develop, understand, and unify their previous, or concurrent, expeditions into chemical theory. (Hochstrasser, 1966)

The author includes three detailed chapters presenting important group theory concepts which then lead to chemical applications. These chapters had the following topics:

- The $C_{n,}$ C_{nv}, C_{nh}, S_n, $D_{n,}$ D_{nd}, and D_{nh} Groups
- Homomorphism
- Isomorphism
- Subgroups
- Invariant Subgroups
- Left and Right Cosets
- Factor Groups
- Characters and classes
- Reducible representations of groups
- Permutation Groups
- Internal Direct Product
- External Direct Product
- Linear Operators

Coupled with every mathematical concept is a directly relevant chemical example. More often than not, each concept is explained not only with a detailed definition and chemical relevance, but also with some sort of accompanying graphic. This text certainly requires no advanced math background and only a rather basic understanding of chemistry as well.

4.1.3 Symmetry through the Eyes of a Chemist (Hagittai, 1986)

István and Magdolna Hargittai, Hungarian Academy of Sciences, Belfast, Hungary

Symmetry through the Eyes of a Chemist is an Inorganic Chemistry textbook used by many different universities including ones as prestigious as Princeton University. The authors are members of the Hungarian Academy of Sciences' Structural Chemistry Research Group. The main focus of this text is to present principles of inorganic chemistry specifically molecular and orbital structure. Unlike previous texts, this book only dedicates a small portion to

presenting useful mathematical concepts such as group theory. In fact there is only one chapter, the fourth chapter that deals with the relevance of group theory to chemical and molecular symmetry. This chapter is titled *Helpful Mathematical Tools* and looks at the following group theory topics: groups, representation of groups, character tables, and direct product. The chapter opens by stating:

> So far our discussion has been non-mathematical. Ignoring mathematics, however, does not make things necessarily easier. Group theory is the mathematical apparatus for describing symmetry operations. It facilitates the understanding and use of symmetries. It may not even be possible to successfully attack some complex problems without the use of group theory. (Hagittai, 1986)

Despite the fact that this text dedicates little attention to the chemical applications of group theory, this chapter still presents all the basic elements of group theory along with some basic examples relating to molecular structure. Without a doubt a course that centers on this text alone could not feature a thorough presentation of the chemical applications of group theory.

4.1.4 **Group Theory and Symmetry in Chemistry** (Hall, 1969)

Lowell H, Hall, Eastern Nazarene College, Quincy, MA

Group Theory and Symmetry in Chemistry presents the powerful relation between group theory and chemistry. The author doesn't spend a great deal of time laying down the fundamentals of group theory yet instead discusses its relevance and importance to chemistry. When needed, he introduces specific definitions and important concepts of group theory. The author states the following provision about the organization of his book:

> Because of the systematic nature of group theory we shall use this abstract theory as the basis for organizing our notions concerning symmetry, as a means not only of developing useful equations but also classifying shapes, functions, and molecular structure. (Hall, 1969)

The presentation and organization of this book is near perfect. While other similar texts introduce group theory and its applications at random points throughout, this text never loses its focus and constantly presents specific mathematical concepts with their respective chemical applications. Although he never gives his own opinion on the demographic he is looking to educate, (undergraduate, graduate, researcher, etc.) Hall only makes chemistry-related assumptions. An advanced math background does not seem expected with this text however, it is very clear that a strong chemistry background along with basic college level mathematics is assumed.

4.1.5 **Group Theory in Chemistry and Spectroscopy** (Tsukerblat, 1994)

Boris S. Tsukerblat, Academy of Sciences of Moldova, Moldova

Group Theory in Chemistry and Spectroscopy is a chemistry text book that looks specifically at the chemical applications of group theory however it does not spend any time establishing basic definitions of group theory as the other texts have. According to the author:

> The physical and chemical applications of group theory are usually based on the geometric symmetries of atoms, molecules and crystals, as well as on the symmetries for the equations describing the properties and behavior of the physical system under consideration. For a contemporary chemist, group theory is not only a key element of the quantum mechanical methods of investigating the electronic structure of matter…The present work is intended as a handbook on group theory for chemists… (Tsukerblat, 1994)

Despite not having a great deal of fundamental concepts of group theory, this book is presented in an advanced mathematical language while still being an advanced chemistry text. The author interweaves advanced mathematical concepts with chemical applications throughout while still maintaining pertinent visual examples to help convey those concepts.

4.1.6 **Molecular Symmetry and Spectroscopy** (Bunker, 1979)

Phillip R. Bunker, Herzberg Institute of Astrophysics, Ottawa, Canada

Molecular Symmetry and Spectroscopy is a very theoretical text that delves more into the mathematics involved in molecular symmetry. According to the author:

> This is a book about the use of group theory in quantum mechanics with particular reference to problems in molecular spectroscopy…The book is aimed at the serious student of molecular spectroscopy, and although knowledge of the postulatory basis of quantum mechanics is assumed, group theory is developed from first principles. The idea of the molecular symmetry group is introduced early in the book (in Chapter 2) after the definition of the concept of a group by using permutations. (Bunker, 1979)

This concept of the molecular symmetry group, which the author denotes as MS, is quite interesting because it is a very comprehensible application of a group theory concept. Specifically, the author uses permutations to help represent symmetry operations.

4.1.7 **The International Encyclopedia of Physical Chemistry and Chemical Physics** (McWeeny, 1963)

The International Encyclopedia of Physical Chemistry and Chemical Physics is a worldwide respected series of texts in mathematics, physics, and chemistry focusing primarily on the latter two. Collectively, the series has over 70 authors and editors all of whom are highly educated and established members of academia spanning from all over the world including: England, Australia, Scotland, the United States, Russia, France, Ireland, the Netherlands, Japan, Canada, Belgium, Germany, and Brazil. According to the introduction:

> The International Encyclopedia of Physical Chemistry and Chemical Physics is a comprehensive and modern account of all aspects of the domain of science between chemistry and physics, and is written primarily for the graduate and research worker. The Editors-in-Chief, Professor E.A. Guggenheim, Professor J.E. Mayer and Professor F.C. Tompkins, have grouped the subject matter in some twenty groups (General Topics), each having its own editor. The complete work consists of about one hundred volumes… (McWeeny, 1963)

The third volume of the first group of general topics, *Mathematical Techniques,* is titled *Symmetry - An Introduction to Group Theory,* written by R. McWeeny from the University of Keele, England. Although this series is by in large dedicated to chemistry and physics, this text primarily presents important concepts in advanced mathematics. This is only appropriate since mathematics is inextricably linked to both fields. In the preface the author is very profound in stressing the importance of group theory to physical chemistry:

> The value of group theoretical methods is now generally accepted. In chemical physics alone, the symmetries of atoms, molecules, and crystals are sufficient to determine the basic selection and intensity rules of atomic spectra, and of the electronic, infra-red and Raman spectra of molecules and crystals…The present book is intended primarily for physics and chemistry graduates who possess a fair amount of mathematical skill but lack the formal equipment demanded by the standard texts. Accordingly, the elementary ideas of both group theory and representation theory are developed in a leisurely but reasonably thorough way, to a point at which the reader should be able to proceed easily to more elaborate applications…Much of the material in this book has been presented to final year undergraduates and to graduate students in the Departments of Mathematics, Physics, and Chemistry at the University of Keele… (McWeeny, 1963)

At first glance, the title would suggest that this is a chemistry text however it is classified in the WPI library as a mathematics text and it's not difficult to see why. Although the author has several applications to physical chemistry, a large portion of the text is dedicated to presenting all the basic concepts of group and representation theory such as:

- Symbols and the group property
- Definition of a group
- Powers, products, generators
- Subgroups, cosets, classes
- Invariant groups and the factor group
- Homomorphisms and Isomorphisms
- The direct product
- The algebra of a group

The author presents a few chapters on specific applications as well. The theorems and mathematics are presented in a very basic yet detailed way that would assume a college education however not necessarily an immense knowledge of abstract algebra and group theory.

Regardless, this text is still extremely advanced in both mathematics and chemistry and it is clear that the author is an expert in both. The author is well versed of the depth of the topic and stresses the importance group theory has to quantum chemistry.

4.2 Chemistry in Group Theory Texts

Research into how chemistry is applied to group theory throughout academia did not yield an equal wealth of information as in the previous section. However, despite the lack of group theory classes addressing applications to chemistry there were still a great deal of related published texts.

4.2.1 **Group Theory and Its Physical Applications** (Falicov, 1966)

L.M. Falicov, University of Chicago, Chicago, Illinois

Group Theory and Its Physical Applications is a text comprised of lecture notes from a graduate course from the Physics Department of the University of Chicago during the summer term of 1964. According to the author:

> They [lecture notes] do not comprise a complete book or a significantly new research contribution to the field; they simply contain a selection of topics in the theory of groups and its application to physical problems… (Falicov, 1966)

This text is unique because it is a composition of physics notes with its primary topics being mathematics and chemistry also. This is due to the fact that book presents "topics that strongly reflect the point of view and personal taste of the author." (Falicov, 1966)

With regards to the chemical applications of group theory, the author has one chapter titled *Applications to Crystal and Molecular Symmetry*. This chapter begins by reintroducing the properties of groups that are relevant to this field of study. These include: the group of all rotations about a given axis, the group of translations, the point groups of the crystal, proper

rotations, reflections, and inversions. The chapter is equally comprised of both mathematical and chemical concepts and never lost focus of the links between the two.

4.2.2 **Applications of Finite Groups** (Lomont, 1959)

J.S. Lomont, New York University, New York

Applications of Finite Groups is a textbook that was used at New York University to present specific applications of group theory to chemistry. Although the text does take a few pages to introduce the fundamental concepts of group theory, the vast majority is dedicated to its applications. According to the author:

> The objectives of this book are: (1) to provide a mathematical background (primarily representation theory) in finite groups which is adequate for both reading this book and for reading the physics literature, and (2) to provide a variety of instructive and interesting examples of applications of finite groups to problems in physics. It is assumed that the reader has been exposed to matrix theory and general group theory. Also, a knowledge of quantum mechanics is presupposed. (Lomont, 1959)

There are two chapters dedicated to applications of group theory including: molecular vibrations, crystallographic point groups, proportionality tensors in crystals, lattice harmonics, and molecular orbitals. The mathematics presented is extremely advanced and more related to physics than chemistry however the text does offer chemical examples relating to molecular symmetry in the section on molecular orbital (MO) theory. The chemistry presented in this section is extremely introductory and does not have any assumptions about the chemical background of the reader. However, the chapters on applications are much more physics related specifically pertaining to tensors. Overall, this is a valuable text for advanced students looking to learn more about applications of group theory.

4.2.3 **Group Theory and Its Applications** (L.C. Biedenharn, 1971)

Numerous Contributors

Group Theory and Its Applications is a series of three volumes written by numerous contributors ranging from the United States, Canada, Sweden, Switzerland, and Mexico. Both the first two volumes have sections dedicated to the chemical applications of group theory. In the first volume there is chapter titled *Group Theory in Atomic Spectroscopy* which is written by B.R. Judd from Johns Hopkins University in Baltimore, Maryland. This chapter deals will many different chemical applications and according to the author:

> Group Theory plays two roles in atomic spectroscopy. Its most obvious function is to take advantage of the symmetry possessed by the Hamiltonian for the electrons of an atom…The rotation group in three dimensions, $O^+(3)$, enters in a direct and physically significant way. It underlies the theory of angular momentum (l), and is central to those applications of group theory to atomic spectroscopy… (L.C. Biedenharn, 1971)

The only major difference between this chapter and others from group theory texts is that this author looks at the symmetries on the atomic level as opposed to the molecular level. Overall the chapter is very abstractly written, as most group theory material is, and does not have any examples or applications. Rather, the author mentions which areas these concepts can be applied to chemistry.

In the second volume, chemical applications are very briefly touched upon in the chapter *Symmetry and Degeneracy* by Harold V. McIntosh from Instituto Politécnico Nacional, Mexico. Specifically the author addresses the symmetries of the hydrogen atom from a mathematical perspective. Virtually no chemistry is presented. Overall, this series is a tremendous resource for students studying advanced math, specifically abstract algebra and group theory, however the text does a very poor job in presenting examples to help demonstrate these applications.

Chapter 5: Chemistry in Mathematics

Burnside Rings: Application to Molecules of Icosahedral Symmetry (Torres, 2004) *Emilio Martínez Torres*, University of Castilla-La Mancha, Spain

In this paper the author begins by stating:

> This paper describes basic facts about this algebraic structure and develops some applications in chemistry, as the labeling of atoms in molecules of high symmetry and the construction of symmetry-adapted functions. For illustrating such applications, the concept of Burnside ring is applied to the icosahedral symmetry. (Torres, 2004)

William Burnside is credited as one of the first contributors to the theory of finite groups. One of his principal contributions to the field is known as Burnside's lemma, also referred to as the Orbit-Counting Theorem. To understand Burnside's lemma, it is important to define a *group action:*

If G is a group and X is a set, then a *(left) group action* of G on X is a binary function

$G \times X \longrightarrow X$ denoted $(g, x) \longmapsto gx;$ which satisfies the following two axioms:

1. $(gh)\cdot x = g\cdot(h\cdot x)$ for all g, h in G and x in X
2. $e\cdot x = x$ for every x in X (where e denotes the identity element of G)

Likewise we also have to define an *orbit:*

Consider a group G acting on a set X. The *orbit* of a point x in X is the set of elements of X to which x can be moved by the elements of G. The orbit of x is denoted by Gx:

$$Gx = \{g \cdot x \mid g \in G\} .$$

Lastly we must define a *fixed point.*

Given a group G and a set X, a fixed point is an element $x \in X$ such that for any $g \in G$:

$$G_x = \{g \in G \mid g \cdot x = x\}.$$

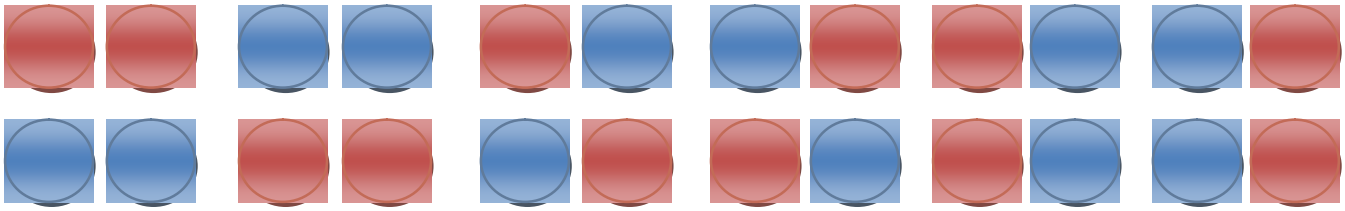
Burnside's lemma states that for a finite group G that *acts* on the set X:

For each g in G let X^g represent the set of fixed points in X. The number of orbits, denoted $|X/G|$, is:

$$|X/G| = \frac{1}{|G|} \sum_{g \in G} |X^g|.$$ (Burnside's Lemma)

Thus, the number of orbits is equal to the average number of points fixed by G.

A simple counting problem is looking at how many distinct ways a necklace can be assembled using two red beads and two blue beads. More specifically, how many ways can the necklace be arranged so that no two arrangements are a rotation of one another. For this example we have three critical assumptions: we assume that there is no clasp to this necklace, allowing us to perform rotations, and we assume that two beads of the same color are indistinct and that the beads are symmetric spheres, so we can include reflections. Given these assumptions, there are six possible bead arrangements:



(1) (2) (3) (4) (5) (6)

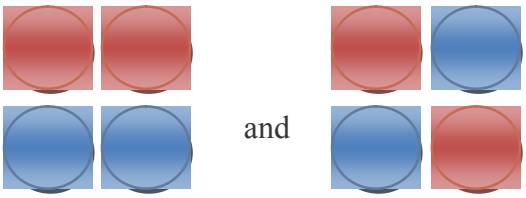
We denote the set X as the set of these six arrangements. The group we are concerned with for this particular problem is the symmetry group of the square, the dihedral group denoted D_4. D_4 has eight elements, and is thus of order 8, that alter the position of the beads. Since the total number of orbits has to be a nonnegative integer, it is essential that the total number of fixed elements is a multiple of the order of D_4. As such, our answer has to be a multiple of 8. Now we look at how the elements of D_4 act on X:

1. *Identity Operation:* Fixes all six arrangements therefore the operation has 6 fixed points.
2. *90 ° counterclockwise rotation:* Changes all six thus the operation has 0 fixed points.
3. *180° counterclockwise rotation:* (3) and (4) remain unchanged so the operation has 2 fixed points.
4. *270° counterclockwise rotation:* Changes all six therefore there are 0 fixed points.
5. *Reflection (about a central vertical axis):* (1) and (2) remain unchanged so the operation has 2 fixed points.
6. *90° Rotation-Reflection:* (3) and (4) remain unchanged so the operation has 2 fixed points.
7. *180° Rotation-Reflection:* (5) and (6) remain unchanged so the operation has 2 fixed points.
8. *270° Rotation-Reflection:* (3) and (4) remain unchanged so the operation has 2 fixed points.

Now applying Burnside's lemma to calculate the total number of orbits, which in this problem are the number of distinct ways the necklace that can be assembled, we see:

$$\text{\# of distinct necklaces} = 1/8*(6+0+2+0+2+2+2+2) = 16/8 = 2$$

Therefore using four beads and two colors, we can only make two distinct necklaces. This is fairly easy to see since intuitively we can only differentiate them by alternating colors or grouping colors:



A more complex example is looking at the rotationally distinct colorings, using five colors, of the faces of the solid cube. Since we have five choices of color for each of the six faces of the cube, we have 5^6 (15,625) possible colored cubes. We denote this set of fixed color cubes *X*. Therefore, we also define *G* as the rotation group for the cube. Along with the identity operation, we have three pairs of faces that rotate three ways, six pairs of edges that rotate one way, and four pairs of corners that rotate two ways; we have 3*3 + 6*2 + 4*2 + 1 = 24 rotations. More specifically, *G* has one identity operation, six 90º face rotations about the axis through the

center of the face and the center of the opposite face, three 180º face rotations about the axis through the center of the face and the center of the opposite face, eight 120º corner rotations about an axis through opposite vertices (a main diagonal), and six 180º rotations about the axis through the midpoint of opposite parallel edges that are not on the same face. These elements perform the following actions on X

1. *One identity operation:* fixing all 15,625 elements of X.
2. *Six 90º face rotations:* This operation fixes two opposite faces of the cube. Therefore all other four faces will have to be one color. The two fixed faces are free. Therefore, the cube will have at most 3 different colors. Therefore 5^3 (125) elements of X are fixed.
3. *Three 180º face rotations:* This operation also fixes two opposite faces of the cube. For the other four faces, we will have two pairs each with their own color. Therefore, we now will have at most 4 colors and 5^4 (625) elements of X are fixed.
4. *Eight 120º corner rotations:* This operation rotates around a main diagonal. Since each vertex touches three faces then there can only be one color for each group of three faces. Since there are two such groups, the cube can have at most 2 colors and thus 5^2 (25) elements of X are fixed.
5. *Six 180º edge rotations:* This operation rotates the cube edgewise. As such each pair of opposite faces must be the same color. Since there are three pairs of opposite faces, there are at most three colors and 5^3 (125) elements of X are fixed.

Using Burnside's lemma to compute the number of orbits of the action of G on X:

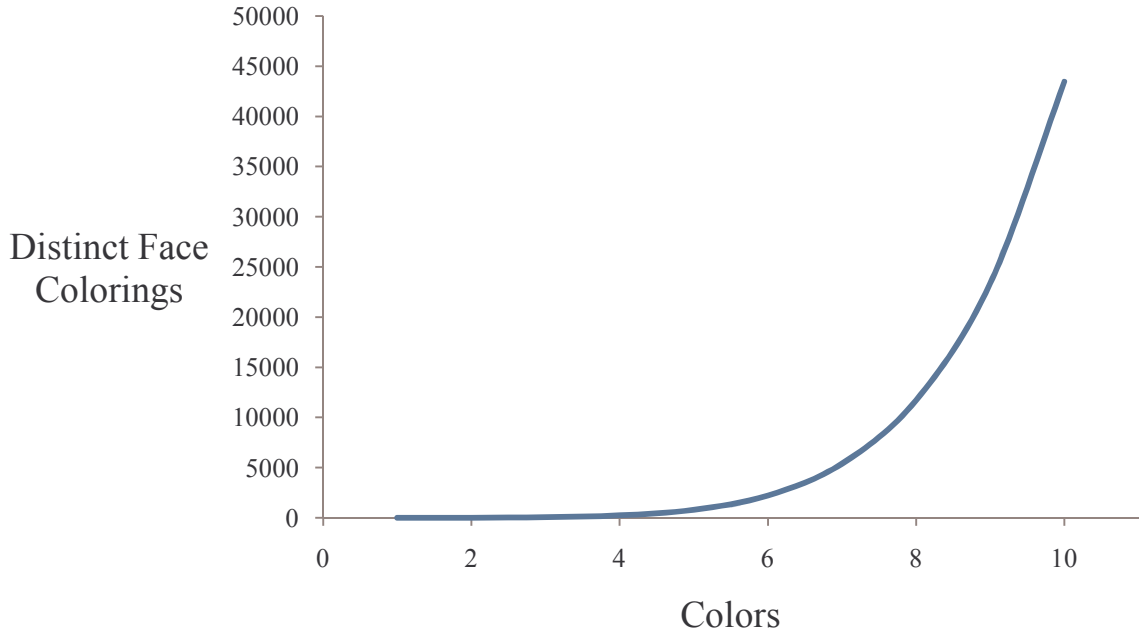
$$|X/G| = (1/24)^* (15{,}625 + 6^*125 + 3^*625 + 8^*25 + 6^*125) = 19{,}200/24 = 800$$

Therefore, there are 800 rotationally distinct colorings of the faces of a cube using six colors and in general using k colors:

$$|X/G| = (1/24)^*(k^6+6k^3+3k^4+8k^2+6k^3)$$

Computing the number of distinct face colorings for different values of k:

Colors (k)	Distinct Face Colorings ($\lvert X/G \rvert$)
2	10
6	2,226
10	43,450
50	651,886,250
100	41,679,670,000



This shows that as the number of colors increases, the number of distinct face colorings increases at an exponential rate. Although the first example was easy to visualize and did not require Burnside's lemma to solve, the second example showed how the same principle could be applied to a much more difficult problem that is certainly not as easy to visualize.

More recently, Burnside's ideas have been applied to algebraic ring structure. A ring, denoted $(R, +, x)$ is a set with two binary operations, addition (+) and multiplication (x), satisfying the following axioms:

(i) $(R, +)$ is an abelian group. This means that + is commutative so that for all $a,b \in R$, $a + b = b + a$.
(ii) x is associative: for all $a,b,c \in R$ $(a \times b) \times c = a \times (b \times c)$
(iii) The distributive laws hold in R: for all $a,b,c \in R$
$(a + b) \times c = (a \times c) + (b \times c)$ and $a \times (b + c) = (a \times b) + (a \times c)$

Mathematically, the author defines the Burnside ring:

Let G be a finite group. The set S is said to be a G-set if to each $g \in G$ and each $x \in S$ there corresponds an element $gx \in S$, such that $1x = x$ (where 1 is the identity element of G) and $f(hx) = (fh)x$ for all $f, h \in G$. Two G-sets S and T are isomorphic with respect to the group action (denoted by $S \cong T$) if there exists a bijection $\varphi: S \rightarrow T$ such that $g\varphi(x) = \varphi(gx)$ for all $x \in S$ and $g \in G$. For each element x in S, its orbit $Gx = \{gx: g \in G\}$ is the smaller G-set containing x. Two elements x and y of S belong to the same orbit if there exists an element g of G such that $y = gx$. Every G-set S can be partitioned into a disjoint union of orbits. A G-set consisting of a single orbit is called transitive.

The stabiliser Gx of an element x of S is the subset of G which fix x, i.e., $Gx = \{g \in G: gx = x\}$. For any $x \in S$, the stabiliser Gx is a subgroup of G. If x and y are two elements of S belonging to the same orbit, the stabilisers Gx and Gy are conjugated subgroups, $Gy = gGxg-1$, where $y = gx$. The stabilisers of the elements of an orbit form a complete conjugacy class of subgroups of G. For any subgroup H of G, the set of left cosets of H in G, given by $G/H = \{gH: g \in G\}$, is a transitive G-set under the G-action given by $f(gH) = (fg)H$. In this case, the stabiliser of gH is $gHg-1$. For any element x of a G-set S the orbit of x is isomorphic to G/Gx. Let H and K be subgroups of G, the sets G/H and G/K are isomorphic G-sets if and only if H and K are conjugated subgroups. Let $\Omega = \{G_1(= \{1\}), G_2, G_3, \ldots, G_s(= G)\}$ be a full set of

nonconjugated subgroups of G. The set of transitive G-sets $\{G/G_i: i = 1, 2, \ldots, s\}$ is a complete set of orbits. This means that every G-set S is isomorphic to a disjoint union of such orbits:

$$S \cong \bigcup_i^{\bullet} a_i(G/G_i), \quad (1)$$

where G_i ranges over all elements of Ω and a_i is the number of times that the orbit G/G_i appears in the decomposition of S. The coefficients a_i are uniquely determined and can be obtained as solutions of the system of linear equations:

$$\sum_{i=1}^{s} M_{ij} a_j = b_j, \quad j = 1, 2, \ldots, s. \ (2)$$

Here M_{ji} is the number of elements in G/G_i which are fixed points of the subgroup G_j, and b_j is the number of elements in S which are fixed points of G_j, where both G_i and G_j run through the set Ω. The square matrix of dimension s formed by the numbers M_{ji} is called the table of marks of the G group. This matrix is nonsingular; hence we can to obtain its inverse M^{-1} which is known as the Burnside matrix. From equation (2) we obtain:

$$a_i = \sum_{j=1}^{s} (M^{-1})_{ij} b_j, \quad i=1,2,3,\ldots,s. \ (3)$$

where $(M^{-1})_{ij}$ is the ij^{th} entry of M^{-1}.

Let S and T be two G-sets. The Cartesian product of S and T, denoted by $S \times T$, is the set of all ordered pairs (x, y) where $x \in S$ and $y \in T$; i.e., $S \times T = \{(x, y): x \in S, y \in T\}$. The action of G on $S \times T$ is given by $g(x, y) = (g(x), g(y))$, for any $g \in G$ and any $(x, y) \in S \times T$. Since $g(x) \in S$ and $g(y) \in T$, $S \times T$ is a G-set. The Cartesian product of the G-sets G/G_i and G/G_j is a G-set, then it is isomorphic to a disjoint union of orbits:

$$(G/G_i) \times (G/G_j) \cong \bigcup_k^{\bullet} n_{ij,k}(G/G_k) \ (4)$$

where G_k ranges over all elements of Ω. If G_l is a subgroup of G the number of fixed points of G_l in G/G_i and G/G_j are M_{li} and M_{lj}, respectively. Then the number of fixed points of G_l in $(G/G_i) \times (G/G_j)$ is $M_{li}M_{lj}$. By applying equation (3), we obtain:

$$n_{ij,k}=\sum_l (M^{-1})_{kl} M_{li} M_{lj}. \quad (5)$$

The Burnside ring $B(G)$ of the group G is defined by:

$$B(G) = \{\sum_{i=1}^{s} a_i (G/G_i) : a_i \in \mathbf{Z}\}, \quad (6)$$

where **Z** is the set of integer numbers. The Burnside ring is a commutative ring with identity G/G_s, where the sum $(G/G_i) + (G/G_j)$ is the disjoint union of G/G_i and G/G_j, and the product $(G/G_i) \cdot (G/G_j)$ is the Cartesian product of G/G_i and G/G_j, i.e.,

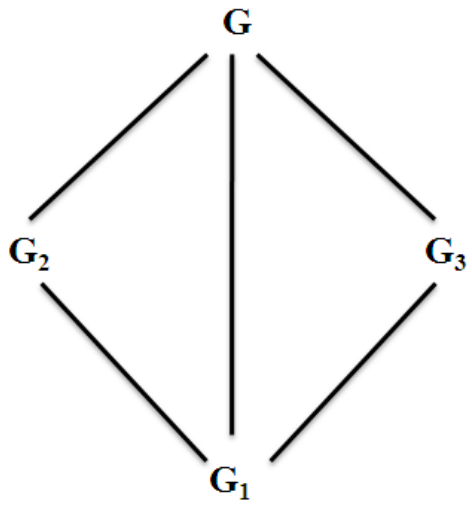
$$(G/G_i) + (G/G_j) = (G/G_i) \cup^{\bullet} (G/Gj),$$

$$(G/G_i) + (G/G_j) = (G/G_i) \text{ x } (G/G_j). \quad (7) \text{ (Torres, 2004)}$$

As an example we generate the Burnside ring corresponding t the symmetric group S_3. We denote S_3 by G. G has six elements, $\{e, r, r^2, s, rs, r^2s\}$. The next step is to determine the subgroups of G:

- $\{e\} = G_1$ (the trivial subgroup)
- $\{e, s\}$, $\{e, rs\}$, $\{e, r^2s\} = G_2$ (these subgroups are each isomorphic to the cyclic group Z_2 since a reflection followed by a relfection is the identity operation)
- $\{e, r, r^2\} = G_3$ (this subgroup is isomorphic to the cyclic group Z_3 since three rotations is the identity operation)
- $\{e, r, r^2, s, rs, r^2s\} = G_4 = G$ (every group is also a subgroup of itself)

From this we can contruct the subgroup lattice of G:



For this example, we are concerned with the set $\{G/G_1, G/G_2, G/G_3, G/G_4\}$ where $G/H = \{gH \mid g \in G\}$:

1. $\boldsymbol{G/G_1} = \{ \{e\}, \{r\}, \{r^2\}, \{s\}, \{rs\}, \{r^2s\} \}$
2. $\boldsymbol{G/G_2} = \{e, r, r^2\} * \{e,s\} = \{ \{e,s\}, \{r,rs\}, \{r^2,r^2s\} \}$
3. $\boldsymbol{G/G_3} = \{e,s\} * \{e, r, r^2\} = \{ \{e, r, r^2\}, \{s,rs, r^2s\} \}$
4. $\boldsymbol{G/G_4} = G/G = \{ \{e, r, r^2, s, rs, r^2s\} \}$

Now we are concerned with how each of the subgroups of G act on each of these sets. Now we introduce *marks* which help to simplify the Burnside ring. A mark is defined as the following:

> Given a group G that acts on a set X, and a group H that is a subgroup of G, then the mark of H on X is the number of elements of X that are fixed by every element of X: $m_X(H) = |X^H|$ where $X^H = \{x \in X \mid h \cdot x = x, \forall h \in H\}$. (Burnside Ring)

Therefore the mark of a product $G_i * (G/G_j)$ is equal to the total number of fixed points. Collectively, all possible marks form a table known as *Burnside's Table of Marks* which is an n x n nonsingular (and therefore invertible) matrix. (Burnside, 1897). Specifically, how many fixed points there are for each group action:

1. $\boldsymbol{G/G_1}$: $\{ \{e\}, \{r\}, \{r^2\}, \{s\}, \{rs\}, \{r^2s\} \}$
   - *(i)* $G_1 * (G/G_1)$: $e * \{ \{e\}, \{r\}, \{r^2\}, \{s\}, \{rs\}, \{r^2s\} \} = \{ \{e\}, \{r\}, \{r^2\}, \{s\}, \{rs\}, \{r^2s\} \}$; therefore we have 6 fixed points.
   - *(ii)* $G_2 * (G/G_1)$: $s * \{ \{e\}, \{r\}, \{r^2\}, \{s\}, \{rs\}, \{r^2s\} \} = \{ \{s\}, \{sr\}, \{sr^2\}, \{e\}, \{srs\}, \{sr^2s\} \}$; therefore we have 0 fixed points.
   - *(iii)* $G_3 * (G/G_1)$: $r * \{ \{e\}, \{r\}, \{r^2\}, \{s\}, \{rs\}, \{r^2s\} \} = \{ \{r\}, \{r^2\}, \{e\}, \{rs\}, \{r^2s\}, \{s\} \}$; therefore we have 0 fixed points.
   - *(iv)* $G_4 * (G/G_1)$: Every element of G/G_1 changes therefore there are 0 fixed points.

Therefore the first row of our table of marks is: [6,0,0,0]

2. ***G/G₂*****:** $\{ \{e,s\}, \{r,rs\}, \{r^2,r^2s\} \}$

   (i) G_1*(G/G_2): trivially we have 3 fixed points.

   (ii) G_2*(G/G_2): $s * \{ \{e,s\}, \{r,rs\}, \{r^2,r^2s\} \} = \{ \{e,s\}, \{sr,srs\}, \{sr^2,sr^2s\} \}$; therefore we have 1 fixed point.

   (iii) G_3*(G/G_2): $r * \{ \{e,s\}, \{r,rs\}, \{r^2,r^2s\} \} = \{ \{r,rs\}, \{r^2,r^2s\}, \{e,s\} \}$; therefore we have 0 fixed points.

   (iv) G_4*(G/G_2): Every element of G/G_2 changes therefore there are 0 fixed points.

Therefore the second row of our table of marks is: [3,1,0,0]

3. ***G/G₃*****:** $\{ \{e, r, r^2\}, \{s,rs, r^2s\} \}$

   (i) G_1*(G/G_3): trivially we have 2 fixed points.

   (ii) G_2*(G/G_3): $s * \{ \{e, r, r^2\}, \{s,rs, r^2s\} \} = \{ \{s, sr, sr^2\}, \{e, r, r^2\} \}$; therefore we have 0 fixed points.

   (iii) $G_3 * (G/G_3)$: $r * \{ \{e, r, r^2\}, \{s,rs, r^2s\} \} = \{ \{r, r^2,e\}, \{rs, r^2s,e\} \}$; therefore we have 2 fixed points.

   (iv) $G_4 * (G/G_3)$: Every element of G/G_3 changes therefore there are 0 fixed points.

Therefore the third row of our table of marks is: [2,0,2,0]

4. ***G/G₄*****:** $G_4 = G$ therefore $G/G_4 = G/G = \{ \{e, r, r^2, s, rs, r^2s\} \}$

   (i) G_1*(G/G_4): trivially we have 1 fixed point.

   (ii) G_2*(G/G_4): $s * \{ \{e, r, r^2, s, rs, r^2s\} \} = \{ \{s, sr, sr^2, e, r, r^2\} \}$ therefore we have 1 fixed point.

   (iii) G_3*(G/G_4): $r * \{ \{e, r, r^2, s, rs, r^2s\} \} = \{ \{r, r^2, e, rs, r^2s, s\} \}$; therefore we have 1 fixed point.

   (iv) $G_4 * (G/G_4)$: Again we have 1 fixed point.

   Therefore the fourth row of our table of marks is [1,1,1,1]

We can now produce our table of marks whose values comprise a 4x4 matrix M:

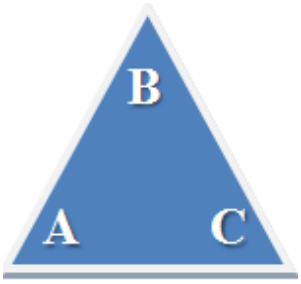
G	G/G_1	G/G_2	G/G_3	G/G_4
G_1	6	3	2	1
G_2	0	1	0	1
G_3	0	0	2	1
G_4	0	0	0	1

Appropriately, this matrix has nonzero entries across the main diagonal; hence we can obtain its inverse M^{-1}:

$$M^{-1} = \begin{pmatrix} 1/6 & -1/2 & -1/6 & 1/2 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & ½ & -1/2 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

This matrix is known as the Burnside matrix. The Burnside ring is defined as the disjoint union of all left cosets G/G_i each with their own coefficient a_i. This coefficient will depend on the particular set we are dealing with.

If we consider an equilateral triangle with each vertex labeled a different letter:



We then denote set X as the set of all the possible triangles we see that for the first vertex we have three choices of letter, the second vertex has two choices, and the third has only one. Therefore, we have 3*2*1= 6 possible triangles. These triangles are all generated by a different element of G acting on the same element of X.

From the Burnside matrix we can compute the coefficients a_i for each coset G/G_i:

$a_i = \sum_{j=1}^{s} (M^{-1})_{ij} b_j, \quad i=1,2,3,\ldots,s.$ *(where* b_j is the number of elements in X which are fixed points of G_j)

We now compute b_j, for j = 1,2,3,4:

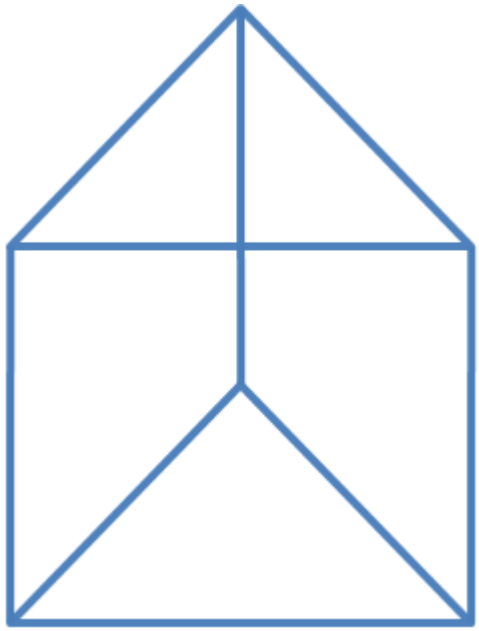
- $b_1 = 6$ (the identity fixes all the triangles)
- $b_2 = 0$
- $b_3 = 0$
- $b_4 = 0$

We now compute the coefficients a_i by multiplying the Burnside matrix M^{-1} by the vector b_j:

$$a_i = \begin{pmatrix} 1/6 & -1/2 & -1/6 & 1/2 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1/2 & -1/2 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 6 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Therefore, for the set X its element of the Burnside ring is the vector $[1,0,0,0]^T$ and more specifcally, this set is congruent to: $\sum_{i=1}^{4} [1,0,0,0] * (G/G_i) = G/G_1 = \{ \{e\}, \{r\}, \{r^2\}, \{s\}, \{rs\}, \{r^2s\} \}$ which we showed was true since each element of G generates one of the six possible triangles.

Letting our group G act on a different set, we now look at a regular triangular prism:



For this example, our set denoted Y is composed of all the elements of the prism:

- 6 vertices (V)
- 5 faces (F)
  - 2 triangular
  - 3 rectangular
- 9 edges (E)
- 1 interior volume (I)

Therefore Y has 21 elements. Now we let the subgroups of G act on Y and count the number of fixed points to get our values b_j:

- G_1: The identity fixes all 21 elements of Y: $b_1 = 21$
- G_2: Z_2 fixes 3 elements of Y ($b_2 = 3$) namely:
  - Both triangular faces
  - The interior volume
- G_3: Z_3 fixes 3 elements of Y ($b_3 = 3$) namely:
  - Both triangular faces
  - The interior volume
- G_4: G fixes 1 element of Y ($b_4 = 1$) namely:
  - The interior volume

So our b_j vector is $[21,3,3,1]^T$. Now we multiply this vector by our Burnside matrix M^{-1} to get our coefficient vector a_i:

$$a_i = \begin{pmatrix} 1/6 & -1/2 & -1/6 & 1/2 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1/2 & -1/2 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 21 \\ 3 \\ 3 \\ 1 \end{pmatrix} = \begin{pmatrix} 2 \\ 2 \\ 1 \\ 1 \end{pmatrix}$$

Therefore, for the set *Y* its element of the Burnside ring is the vector $[2,2,1,1]^T$ and more specifcally, *Y* is congruent to $\sum_{i=1}^{4}[2,2,1,1] * (G/G_i)$ meaning we can express the set *Y* as being congruent to the following sum: $2(G/G_1) + 2(G/G_2) + (G/G_3) + (G/G_4)$.

The generators of the Burnside ring are simply the columns of the table of marks. This ring is commutative with identity element G/G_4 where addition is given by disjoint union and multiplication is given by the Cartesian product:

$$(G/G_i) + (G/G_j) = (G/G_i) \cup^{\bullet} (G/G_j), \textit{ (disjoint union)}$$

$$(G/G_i) * (G/G_j) = (G/G_i) \text{ x } (G/G_j). \textit{ (Cartesian product)}$$

To give an example of what is meant by Cartesian product in this example, we simply look at the rows of our table of marks. We can multiply (G/G_i) x (G/G_j) simply by multiplying the columns component-wise. For example:

$$(G/G_2) \text{ x } (G/G_3) = [3,1,0,0]^T * [2,0,2,0]^T = [3*2,1*0, 0*2, 0*0] = [6,0,0,0]^T = G/G_1$$

We now construct the multiplication table of our Burnside ring $B(G)$:

G	G/G_1	G/G_2	G/G_3	G/G_4
G/G_1	$6(G/G_1)$	$3(G/G_1)$	$2(G/G_1)$	G/G_1
G/G_2	$3(G/G_1)$	$G/G_1 + G/G_2$	G/G_1	G/G_2
G/G_3	$2(G/G_1)$	G/G_1	$2(G/G_3)$	G/G_3
G/G_4	G/G_1	G/G_2	G/G_3	G/G_4

Using this multiplication table we can compute the product of our two sets X and Y. From a physical standpoint this product isn't practical however the product can still be calculated. Recalling that X is congruent to G/G_1 and Y is congruent to $2(G/G_1) + 2(G/G_2) + (G/G_3) + (G/G_4)$ the product X x Y is:

$$\begin{aligned} X \text{ x } Y &= (G/G_1) \text{ x } (2(G/G_1) + 2(G/G_2) + (G/G_3) + (G/G_4)) \\ &= 2(6(G/G_1)) + 2(3(G/G_1)) + 2(G/G_1) + G/G_1 \\ &= 12(G/G_1) + 6(G/G_1) + 2(G/G_1) + G/G_1 \\ &= 21(G/G_1) \end{aligned}$$

Since X has 6 elements and Y has 21 elements, it follows that the product X x Y has 6 x 21 (126) elements. Since we defined G/G_1 to have six elements, $21(G/G_1)$ will have a total of 126 elements and therefore our product is correct.

Choosing $G = S_3$ was a relatively simple example since S_3 has order six. However, no matter what the size of the group or the set on which the groups acts, the procedure is still the same. For these examples, we chose S_3 acting on the set of triangles but we could have chosen S_3 on a much larger set. This demonstrates how the Burnside ring allows you to simplfy and decompose complex geometric structures.

In the paper, the author looks at the icosahedral rotation group I. The icosahedral rotation group I is a subgroup of the icosahedral group I_h which is the group of symmetries of the

icosahedron and is of order 120. *I* is of order 60 and isomorphic to the alternating group A_5 of even permutations of five objects. *I* acts on the icosahedron which is defined as any polyhedron having 20 faces. A regular icosahedron is a platonic solid with faces that are equilateral triangles. A platonic solid is a convex regular polyhedron. A regular icosahedron has 30 edges and 12 vertices with five triangles meeting at each vertex. *I* has a total of five symmetry operations that collectively form the group:

- 1 identity operation (e)
- 12 proper rotations about the C_5 axis (C_5)
- 12 sets of two proper rotations about the C_5 axis (C_5^2)
- 20 proper rotations about the C_3 axis (C_3)
- 15 proper rotations about the C_2 axis (C_2)

Although this group is much more complex than the one we chose, the procedure for generating the ring is exactly the same. The only differences being the number of orbits (*I* has nine distinct orbits), and their cardinalities. The orbits of *I* are the following:

(I) A single point in the origin of coordinates
(T) The set of three orthogonal pairs of antipodal edge midpoints of the icosahedron
(D_5) The set of pairs of antipodal vertices of the icosahedron
(D_3) The set of pairs of antipodal face midpoints of the icosahedron
(D_2) The set of pairs of antipodal edge midpoints of the icosahedron
(C_5) The set of vertices of the icosahedron
(C_3) The set of face midpoints of the icosahedron
(C_2) The set of edge midpoints of the icosahedron
(C_1) The set of vertices of a truncated icosahedron (Torres, 2004)

I generates different platonic including the dodecahedron (12 faces), icosahedron (20 faces), icosidodecahedron (32 faces), small rhombicosidodecahedron (62 faces), and the snub dodecahedron (92 faces). Archimedean solids are defined as highly symmetric polyhedrons that are composed of two or more types of regular polygons meeting at identical vertices. Specifically, *I* generates two different Archimedean solids: the truncated dodecahedron (32 faces), and the truncated icosahedron (32 faces). The truncated icosahedron, the shape used in the design of soccer balls, has identical structure to the molecule C_{60} Buckminsterfullerene,

commonly known as a *buckyball*. Both the truncated icosahedron and Buckminsterfullerene molecule have 20 regular hexagonal faces as well as 12 regular pentagonal faces. Likewise, both have 60 vertices and 90 edges where for C_{60}, each vertex represents an atom and each edge represents a bond.

This knowledge and application of symmetry to molecular structure is critical to chemistry. In the case of C_{60}, it is extremely useful considering the molecule itself was discovered only 23 years ago in 1985:

> Chemists discovered a 60-atom carbon molecule, dubbed buckminsterfullerene, which seems to have a structure with the same geometry as the pattern on a soccer ball. (Science News of the Year, 1985)

As such, there is still much to be learned about the molecule and the fullerene family as a whole. These molecules have a very short half-life and as such are difficult to discover in nature. In fact, the existence of C_{60} was predicted in 1970 by Eiji Osawa of Toyohashi University of Technology, an engineering university in Toyohashi, Aichi, Japan. He was able to make this prediction by looking at the molecule $C_{20}H_{10}$ corannulene. He discovered that corannulene had to be a substructure of larger molecule. Without this observation, it is very possible that buckminsterfullerene might still be undiscovered.

Chapter 6: Mathematics in Chemistry

Group Theory and the Near-Ultraviolet Absorption Spectrum of Gas-Phase Benzene (Bryce E. Williamson, 2002) *Bryce E. Williamson, Kristen C.L. Taylor*, University of Canterbury, Christchurch, New Zealand

ACELL, Australasian Chemistry Enhanced Laboratory Learning, was founded in the late 1990's and initially funded by the Australian government. According to the ACELL website they have three principal aims:

- To make available, via a database, materials relating to undergraduate chemistry experiments which are educationally sound and have been evaluated by both students and academic staff. These materials consist of everything needed to introduce the experiment into another institution, as well as evaluation data relating to both the chemical and the educational aspects of the experiment;
- To provide for the professional development of chemistry academic staff by expanding the understanding of issues surrounding student learning; and,
- To facilitate the development of a community of practice in chemistry education within the broader academic community of the Australasian region. (ACELL, 2002)

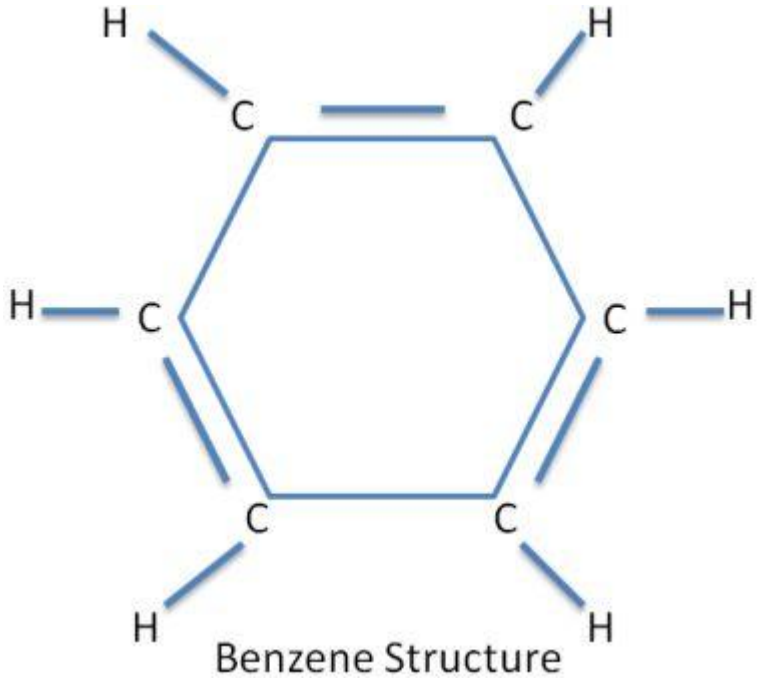
The predecessor to ACELL was APCELL, Australian Physical Chemistry Enhanced Laboratory Learning. APCELL was designed to offer state of the art chemistry laboratories and equipment to thousands of Australian chemistry students. The resources that APCELL provides chemistry students includes a variety of laboratory procedures designed to illustrate the concepts presented in chemistry lectures at the university level.

One of these procedures is titled *Group Theory and the Near-Ultraviolet Absorption Spectrum of Gas-Phase Benzene* (Bryce E. Williamson, 2002). This project is designed to introduce students to how elements of group theory can be applied to further understanding molecular structure and interpreting UV spectral data. The laboratory description of this project reads the following:

> Modern physical models, such as quantum mechanics, provide powerful means by which to describe and rationalise molecular properties. However, as the size (the number of electrons and

> nuclei) of the molecule increases, brute-force treatments employing such models can rapidly expand to ungainly proportions, which make the problem extremely difficult to conceptualise. One way to simplify such problems is to employ the techniques of group theory. Group theory is a branch of mathematics that has a vast number of applications in the physical sciences. In chemistry, it permits aspects of molecular problems to be categorised in terms of molecular symmetry, with a consequent reduction of the apparent complexity. This, in turn, vastly aids the interpretation and conceptualisation of experimental and theoretical data. (Bryce E. Williamson, 2002)

The authors of this laboratory procedure state that benzene (C_6H_6) was chosen "for a number of reasons." (Bryce E. Williamson, 2002) The most important reason being that "benzene is a prototypically simple and relatively symmetric polyatomic molecule…" (Bryce E. Williamson, 2002) Benzene is an organic compound with the following molecular structure:

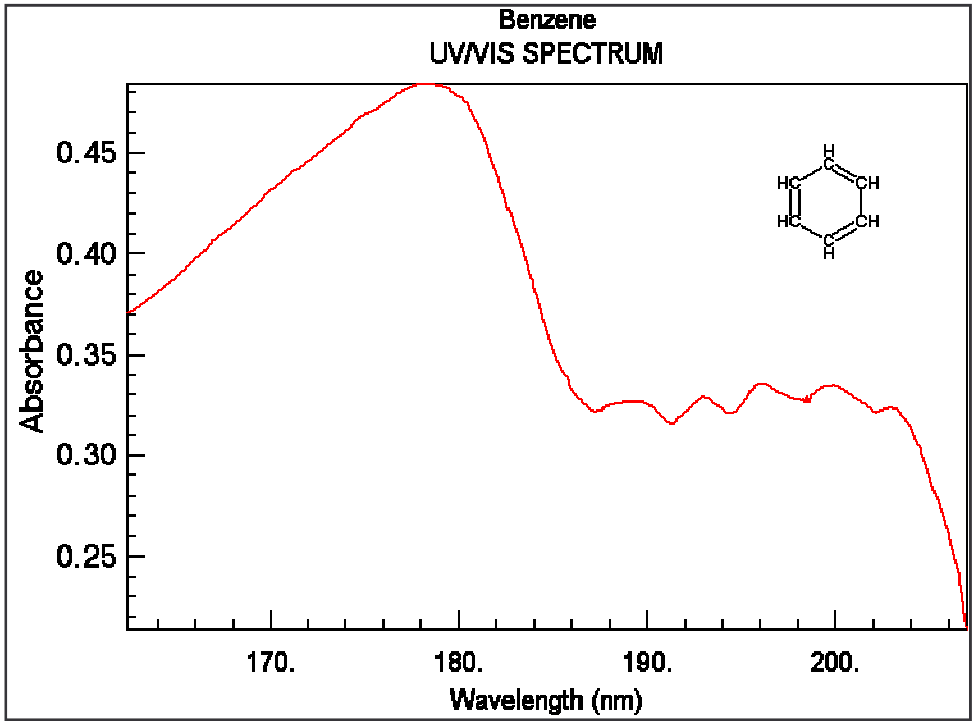


Benzene Structure

Benzene is comprised of six carbon atoms and six hydrogen atoms. This cyclohexene structure contains alternating covalent single and double bonds, as is seen in a conjugated system. As seen in the figure above, each carbon molecule is covalently bonded to a hydrogen atom.

Specifically, this laboratory procedure deals with ultraviolet-visible (UV/VIS) spectroscopy and the absorption spectrum of benzene. UV/VIS spectroscopy is routinely used in

the quantitative determination of solutions of transition metal ions and highly conjugated organic compounds (such as benzene). (Ultraviolet-visible spectroscopy) Photons from the visible spectrum of light specifically near the ultraviolet range are used in UV/VIS spectroscopy. In this range of the visible spectrum, molecules undergo electronic transitions when valence electrons jump from one energy level to a higher energy level giving off a photon. Different molecules absorb light at different wavelengths, depending on the molecular structure. More specifically, the differences in wavelengths depend on the structural subgroups in the molecule. Benzene has the following UV/VIS spectrum:



(UV/VIS Absorption Spectrum of benzene)

The rest of the lab, and the overwhelming majority of it, is dedicated to analyzing this spectrum by applying group theory concepts in order to demonstrate the practical applications of the theorectical concepts.

Bibliography

1. *ACELL*. (2002). Retrieved from http://acell.chem.usyd.edu.au/Current-Project.cfm?obj_id=171
2. Bertolucci, D. H. (1989). *Symmetry and Spectroscopy.* Dover Publications .
3. Bryce E. Williamson, K. C. (2002). *Group Theory and the Near-ultraviolet Absorption Spectrum of Gas-phase Benzene: An APCELL Experiment.* Retrieved from http://acell.chem.usyd.edu.au/ExpDocs/williamsontaylor(2002)_ausjec_v58p13.pdf
4. Bunker, P. R. (1979). *Molecular Symmetry and Spectroscopy.* New York, NY: Academic Press Inc. .
5. *Burnside Ring*. (n.d.). Retrieved from http://en.wikipedia.org/wiki/Burnside_ring
6. Burnside, W. (1897). *Theory of Finite Groups.*
7. *Burnside's Lemma*. (n.d.). Retrieved from http://en.wikipedia.org/wiki/Burnside's_lemma
8. Carter, R. L. (1998). *Molecular Symmetry and Group Theory.* John Wiley and Sons Inc.
9. *Chemistry 104A*. (2007). Retrieved from http://www.cchem.berkeley.edu/pdygrp/chem104a.html
10. *Chemistry 505: Group Theory in Chemistry*. (n.d.). Retrieved from http://www.princeton.edu/~catalase/505_Course%20Outline_99.pdf
11. *Chemistry 673 Symmetry and Group Theory in Chemistry*. (n.d.). Retrieved from http://www.chem.tamu.edu/rgroup/hughbanks/courses/673/chem673syllabus.pdf
12. *Chemistry Courses (CHM)*. (n.d.). Retrieved from http://www.bulletins.wayne.edu/gbk-output/lib12.html
13. *CHM 545 Quantum Chemistry*. (n.d.). Retrieved from http://www.public.asu.edu/~dmatyus/teaching/chm545/chm545.html
14. Cotton, F. (1990). *Chemical Applications of Group Theory.* Toronto, Canada: John Wiley and Sons, Inc.
15. Douglas, B. M. (1994). *Principles and Models of Inorganic Chemistry.* Wiley .
16. *F. Albert Cotton*. (n.d.). Retrieved from http://en.wikipedia.org/wiki/F._Albert_Cotton#_note-mccue
17. Falicov, L. M. (1966). *Group Theory and Its Physical Applications.* Chicago, Illinois: The Univeristy of Chicago Press.
18. Gallian, J. A. (2004). *Contemporary Abstract Algebra 6th Edition.* Houghton-Mifflin.

19. *Graduate Chemistry Courses*. (n.d.). Retrieved from http://www.case.edu/artsci/chem/grad/gcourses.html
20. *Group Action*. (n.d.). Retrieved from http://en.wikipedia.org/wiki/Group_action
21. Hagittai, I. H. (1986). *Symmetry through the Eyes of a Chemist.* New York, NY: VCH Publishers.
22. Hall, L. H. (1969). *Group Theory and Symmetry in Chemistry.* New York, NY: McGraw-Hill.
23. Hochstrasser, R. M. (1966). *Molecular Aspects of Symmetry.* New York, NY: W.A. Benjamin Inc. .
24. L.C. Biedenharn, E. B.-M.-L. (1971). *Group Theory and Its Aplications.* New York, NY: Academic Press, Inc.
25. *Lagrange's Theorem (group theory)*. (n.d.). Retrieved from http://en.wikipedia.org/wiki/Lagrange's_theorem_(group_theory)
26. Lomont, J. S. (1959). *Applications of Finite Groups.* New York, NY: Academic Press Inc.
27. *Massachusetts Institute of Technology Chemistry Department Course Catalog 2007-2008*. (n.d.). Retrieved from http://stellar.mit.edu/S/course/5/fa07/5.04/index.html
28. McWeeny, R. (1963). *The International Encyclopedia of Physical Chemistry and Chemical Physics: Topic 1: Mathematical Techniques Volume 3: Symmetry-An Introduction to Group Theory.* Oxford, England: Pergamon Press Ltd.
29. *Michigan Tech Graduate Course Descriptions 2007*. (n.d.). Retrieved from http://www.admin.mtu.edu/catalog/courses/grad/pdf/ch.pdf
30. Miessler, D. A. (2003). *Inorganic Chemistry 3rd Edition.* Upper Saddle River, NJ: Prentice Hal.
31. Schatz, G. C. (2002). *Quantum Mechanics in Chemistry.* Dover Publications.
32. Science News of the Year. (1985). *Science News* , 403.
33. Sharpe, C. E. (2005). *Inorganic Chemistry 2nd Edition.* Pearson Educated Ltd.
34. Shriver, D. A. (2006). *Inorganic Chemistry.* W.H. Freeman .
35. *Stanford Bulletin: Chemistry Department 2007-2008*. (n.d.). Retrieved from http://registrar.stanford.edu/bulletin/pdf/Chemistry.pdf

36. Torres, E. M. (2004). Burnside rings: Application to molecules of icosohedral symmetry. *Journal of Mathematical Chemistry* , 105-116.
37. Tsukerblat, B. S. (1994). *Group Theory in Chemistry and Spectroscopy.* Oxford, England: Alden Press Ltd. .
38. *UCL Chemistry*. (n.d.). Retrieved from http://www.chem.ucl.ac.uk/admissions/synopses/chem2102.shtml
39. *Ultraviolet-visible spectroscopy*. (n.d.). Retrieved from http://en.wikipedia.org/wiki/Ultraviolet-visible_spectroscopy
40. *UV/VIS Absorption Spectrum of benzene*. (n.d.). Retrieved from http://www.wooster.edu/chemistry/is/brubaker/uv/uv_spectrum.html
41. *WPI Chemistry and Biochemistry Department Coure Catalog 2007-2008*. (n.d.). Retrieved from http://www.wpi.edu/Pubs/Catalogs/Ugrad/Current/chcourses.html#ch3410
42. *WPI Mathematical Sciences Department Course Catalog 2007-2008*. (n.d.). Retrieved from http://www.wpi.edu/Pubs/Catalogs/Ugrad/Current/macourses.html#ma3823