CHEMISTRY 673

Symmetry and Group Theory in Chemistry
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CHEMISTRY 673

Content of the course

Applications of symmetry and group theory to various types of chemical systems; classification of molecules into symmetry point groups and use of character tables.

1. Definitions and Theorems of Group Theory
2. Molecular Symmetry and the Symmetry Groups
3. Crystallographic Symmetry
4. Representations of Groups
5. Vibrational Symmetry
6. Group Theory and Quantum Mechanics
7. Symmetry-Adapted Linear Combinations
8. Molecular Orbital Theory and Its Applications in Organic Chemistry
9. Molecular Orbital Theory for Inorganic and Organometallic Chemistry
10. Ligand Field Theory
Learning Outcomes from Chem 673

* Recognition of molecular symmetry and the symmetry group to which a molecule of known structure belongs.

Practical understanding of crystallographic symmetry

Thorough understanding of what constitutes a group - mathematical representations of groups

Nomenclature of atomic and molecular spectroscopy – how nomenclature relates to symmetry properties

Representing molecular properties such as vibrations, electronic spectra, molecular orbitals

Reading the literature involving symmetry
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» text is well written, at right level
» we follow the text with some handouts and reference materials

Lecture: 2 × 75 min/week; TTh 11:10 - 12:25, Room 2122

This course is for 3 credits.

A WEB site will be available:
http://www.chem.tamu.edu/rgroup/fackler

Grades will be based on the homework (roughly 20%), midterm and final exams
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Prerequisites

Undergraduate chemistry courses, especially inorganic and physical chemistry.

Usual math courses for scientists, especially linear algebra.

If you have not had linear algebra, then familiarity with vectors and matrices acquired elsewhere may suffice — don’t wait to review these topics, do so this week! - Minimum background: Appendix in Cotton’s text.
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Other texts of interest

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- Please try to keep ahead in reading.
- This will allow me to avoid much mathematical detail in class. This is desirable because theorems and proofs become tedious!
- Start with the first 3 chapters now!
Scientific grandfather: Geoffrey Wilkinson
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Why is symmetry and group theory of value?

- All properties of matter must conform to the symmetry of the system.
- Quantum Mechanical solutions must conform.
- Group theory gives us a mathematical representation of these symmetry properties.
What is Group Theory?

- A fairly “recent” branch of mathematics. Early principles were developed by Évariste Galois (killed in a duel in 1832 at age 21), and Niels Abel (died in 1829 at age 26 of TB).
- First formal definition of a group was given by Cayley in 1854. Fedorov pioneered the application of group theory to crystallography.
- Group Theory is the closest many chemists get to truly “modern” mathematics.
Properties of Groups

- Closure: “product” of any two group elements (operations) is a group element (operation), including squares
- One element, the identity, commutes with all others
- Associative property holds (commutative property does not necessarily hold)
- Every element (operation) has an inverse — which is also a group element (operation)
The integers, under the operation of addition?
The integers, under the operation of multiplication?
A simple symmetry group, $C_{2v}$
  – what are the elements (operations)?
  – how do we define a product?
Mathematically, the members of a group are called “elements”

In symmetry groups these “elements” are called “operations” - the term “element” is reserved for something else:

The term “symmetry element” refers to a geometrical entity (a point, a line or axis, or a plane) about which the operation is defined.
Reflection (in a plane) \( \sigma \)
Inversion (through a point) \( i \)
Rotation (about a proper axis) \( C_n \)
- through an angle \( 2\pi/n \)
Improper Rotation (rotation reflection) \( S_n \)
Rotation - Inversion equivalent \( \bar{n} \)
Identity (do nothing) \( E \)