Spectroscopy of Inorganic Compounds

329 Chem. (2+0)

Course Catalogue

Introduction: characterization of electromagnetic radiation, quantization of energy, regions of spectrum, representation of spectrum, basic elements of practical spectroscopy, signal-to-noise, resolving power, width and intensity of spectral lines. Microwave spectroscopy: rotation of molecules, rotational spectra, diatomic molecules. Infra-red spectroscopy: vibrating diatomic molecule, diatomic vibrating rotator, vibration-rotation spectrum of carbon monoxide, breakdown of the Born-Oppenheimer approximation, interaction of rotations and vibrations. Electronic spectroscopy of atoms: structure of atoms, electronic angular momentum, multi-electron atoms, angular momentum of multi-electron atoms. Spin resonance spectroscopy: spin and applied field, nuclear magnetic spectroscopy, electron magnetic spectroscopy. Group Theory: Molecular symmetry and the symmetry groups, symmetry point groups, representation of groups, applications.

Course objectives

This course was designed to offer students a deeper understanding of the concepts behind spectroscopic methods used to characterize inorganic compounds. A non-mathematical approach focusing on fundamental, rather than analytical aspects was adopted, with molecular symmetry in mind. A substantial portion of descriptive chemistry, which requires careful reading *and* retaining of gained knowledge, is included in this class. Examples of interpretation of data of physical methods with regard to structure and properties of the compounds will be investigated independently. IR, ….. Electronic spectroscopy, .

Content and Learning Outcomes

Part I Symmetry and Groups (4 weeks)

Topics: Symmetry, Point Groups, Chirality and Polarity, Groups and Representations, Transformation Matrices, Character Tables, Symmetry Labels.

Outcomes: The student should be able to:

1. *Describe ways in which the symmetry of a molecule can be classified (symmetry elements and symmetry operations).*
2. *Introduce a shorthand notation that embraces all the symmetry inherent in a molecule (a point group symbol).*
3. *Define chirality of a molecule according to its symmetry and point group.*
4. *Apply transformation matrices (to place the concept of symmetry on a more quantitative basis).*

5. *Be able to reach numerical representations for the point group symmetry operations.*
6. *Construct the character table for simple molecules with appropriate symmetry labels.*

Part II : Application of Group Theory to Vibrational Spectroscopy (3 weeks)
Topics: Reducible Representations, The Reduction Formula, The Vibrational Spectrum of SO_2, Chi Per Unshifted Atom, Techniques of Vibrational Spectroscopy, Infrared Spectroscopy, Raman Spectroscopy, Rule of Mutual Exclusion, Stretching and Bending Modes, The Vibrational Spectrum of $Xe(O)F_4$, Group Frequencies.

Outcomes: Student should be able to:
1. *Use techniques learned from of Part I and apply to the analysis of vibrational spectra.*
2. *Predict the vibrational spectrum of the simple molecules using group theory and the demands of point group symmetry.*
3. *Generate a reducible representation of the point group using vectors.*
4. *Convert the reducible representation to the sum of a series of irreducible representations.*
5. *Identify the symmetry labels associated with the molecular vibrations.*
6. *Apply knowledge to the vibrational spectrum of $Xe(O)F_4$*

Part III Application of Group Theory to Structure and Bonding (3 weeks)

Topics: Fundamentals of Molecular Orbital Theory, Bonding in H_2, Bonding in Linear H_3, Limitations in a Qualitative Approach, Symmetry-Adapted Linear Combinations, Central Atom Orbital Symmetries, H_2O – Linear or Angular ? NH_3 – Planar or Pyramidal ? Octahedral Complexes *d*-Orbital Symmetry Labels, Octahedral P-Block Complexes, Octahedral Transition Metal Complexes, π-Bonding and the Spectrochemical Series.
Outcomes: Student should be able to:
1. *Apply the group theory on simple molecules in developing descriptions for bonding patterns.*
2. *Be able to predict symmetries of molecular orbitals from atomic orbitals.*
3. *Extend knowledge in constructing molecular orbitals to more complex molecules.*

Part IV Application of Group Theory to Electronic Spectroscopy (2weeks)

Topics: Symmetry and Selection Rules, Symmetry of Electronic States, Selection Rules, The Importance of Spin, Degenerate Systems, Terms and Configurations, term Symbols, The Effect of a Ligand Field – Orbitals,
d-d Spectra,

Outcomes: Student should be able to:
1. *Applying symmetry to understanding and interpreting electronic spectra*
2. *To describe the way the distribution of electrons in orbitals in terms of symmetry labels*
3. *Using symmetry to determine the selection rules for electronic transitions*

4. *Be able to define the degeneracy of a system using the direct product method and relating it to the symmetry concept.*
5. *Apply built knowledge to electronic spectra of transition metal complexes (d–d electron transitions).*

Delivery and evaluation

- All topics will be delivered through lectures (ppt files on LMS).
- Continuous independent and group problem solving activities, as well as in-class activities (20 marks).
- Workshops to apply what is learned.
- Two midterm exams (40 marks).
- Final exam (40 marks).

References

- G. Davidson, Group theory for chemists, 1991.
- K. C. Colloy, Group theory for chemists; Fundamental theory and applications, 2010.

- Useful link
  http://symmetry.otterbein.edu/
  Animated Symmetry tutorials and gallery

Instructor's Expectations

1. **Attitude**: Attentiveness, seeking help and asking questions when something is not clear or not well understood.
2. **Attendance** is a necessary condition for receiving of solid knowledge of the subject and a good grade. Therefore, all lectures should be attended.
3. The schedule **may be** modified throughout the course, as needed. **And the student is expected to cope.**

Obtaining Assistance Do not hesitate to contact the instructor during office hours or via e-mail.

Instructor's Information

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