Approval: 8th Senate Meeting

Course Name: Group Theory and Spectroscopy

Course Number: CY511

Credits: 3-0-0-3

Prerequisites: B.Sc. (with Chemistry) or Teachers Consent

Intended for: UG/PG

Distribution: Core

Semester: Odd/Even

Course Preamble: The main focus of this course is to provide the students with deeper understanding on spectroscopy. It also emphasis on how molecular symmetry and group theory are usefully related to spectroscopy. In addition, this course also aims to strengthen the knowledge of the students in some fundamental concepts of spectroscopic transition of molecules by combining both spectroscopy and group theory together.

Course Outline:

Unit 1: Molecular symmetry and group theory [16 Lectures]

Definition of a group and basic theorems, Group multiplication table, elements of a symmetry group, symmetry group classification. The Great Orthogonality theorem Direct products, similarity transformation, Characters of representation, Character table, irreducible representation, symmetry adopted linear combination, bonding in diatomics, group theory and molecular electronic states.

Unit 2: Interaction of light with matter [4 Lectures]

Transition moments and transition probabilities, Einstein's coefficients, oscillator strength, Beer-Lambert law, polarizabilities, oscillator strength, relationship between Einstein's coefficients and total absorbance. Born- Oppenheimer approximation, Frank Condon Principles,

Unit 3: Rotational and Vibrational Spectroscopy [16 Lectures]

Moment of inertia, The Rotational energy levels, Rotational spectra of diatomic molecules, Rotational Raman spectra, Rotational spectra of polyatomic molecules, Molecular vibrations, Selection rules, vibrational spectra of diatomic molecules, simple harmonic oscillator and rigid rotor model, anharmonic corrections, Vibrational-Rotational Spectra, vibrational Raman spectra of diatomic molecules. Infrared absorption spectra of polyatomic molecules, symmetric and asymmetric top molecules, normal modes of vibration and their classification by group theory, coupling between rotational and vibrational degrees of freedom. Symmetry and normal modes of vibrations. Symmetry and selection rules for allowed transitions among rotational, vibrational level. Determining the symmetry of molecular motions. Group theory and molecular electronic

transitions. Symmetry and selection rules, spin and parity forbidden transitions, vibronic interaction.

Unit 4: Electronic spectroscopy [6 Lectures]

Electronic angular momentum and magnetic moment, atomic spectroscopy, spectra of hydrogen atom, many electron atoms, spectra and structure of diatomic molecule, electronic spectra of polyatomic molecules

Text Books:

1. Physical Chemistry: A Molecular Approach by Donald A. McQuarrie and John D. Simon, Viva Books, First South Asia Edn. 1998.
2. Physical Chemistry by Peter Atkins and Julio de Paula (Oxford University Press 7th Edn. 2002.
3. Modern Spectroscopy, J. M. Hollas, John Wiley, 4thEdn., 2004.
4. Chemical Applications of Group Theory, F. A. Cotton, John Wiley, 3rd Edn. 2003.

Reference Book:

1. Ira N. Levine, Quantum Chemistry, Prentice-Hall: Englewood Cliffs, NJ, USA (1991).
2. Molecular Symmetry and Group Theory, Alan Vincent, 2nd Edn. Wiley, 2000.
3. Molecular Symmetry and Group Theory by Robert L. Carter. John Wiley & Sons. Inc. New Yowk, 1997.
4. Symmetry and Spectroscopy of Molecules. K. Verra Reddy, New Age International Limited Publishers 2nd End. 2009.