CY701 Advances Physical Methods in Chemistry: Theory and Applications

Credit: 3-0-0-3 Approval: Approved in 1st Senate

Elective or core: Elective

Students intended for: Ph.D.

Prerequisite: Consent of the faculty member Semester: Odd/Even

Course Objective:

To make scientific background stronger in fundamental physical methods in chemistry. Researchers will be benefited for a better understanding of the advanced spectroscopic techniques.

Course contents:

- **Quantum Chemistry and molecular symmetry: (Lecture Hours : 8)** Schrödinger wave equation, Born Oppenheimer Approximation and electronic wave function, particle in a box, potential well, potential barrier and tunneling. Definition of a group and basic theorems, molecular symmetry groups and classes, symmetry and normal modes of vibrations, determining the symmetry of molecular motions, symmetry and selection rules for allowed transitions among rotational, vibrational level, group theory and molecular electronic transitions
- **Interaction of light with matter: (Lecture Hours : 10)** Transition moments and transition probabilities, Einstein's coefficients, oscillator strength, Beer-Lambert law, polarizabilities, Frank Condon Principles, Fluorescence and absorption spectroscopy, Quantum yield and its measurements. Donor_acceptorcomplexes. Fluorescence quenching (static and dynamic). Stern_Volmer analysis.Timescale of molecular processes in solution. Steady_state and time-resolved fluorescence. Fluorescence anisotropy. Biochemical fluorophores. New fluorescence technologies: Multiphoton Excitation, Fluorescence correlation Spectroscopy, Single molecule detection.
- **Rotational and Vibrational Spectroscopy: (Lecture Hours : 7)** Moment of inertia, The Rotational energy levels, Rotational spectra of diatomic molecules, Rotational Raman spectra, 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.
- **Nuclear Magnetic Resonance Spectroscopy: (Lecture Hours :10)** Basic Principles, Chemical shifts, Spin_spin interactions. Application of 1H and 13CNMR spectroscopy including COSY, NOESY in the structure determination of bioorganic compounds. Application in conformational analysis. Solid state NMR.Instrumental aspects. Multinuclear NMR of various inorganic and organo_metalliccompounds. Instrumental aspects.
- **Mass spectrometry: (Lecture Hours :5)** Basic concepts. Fragmentation and rearrangements (including McLaffertyre arrangement) of different classes of organic molecules. Isotope effect. ESI_MS, MALDI_TOF techniques.

Text Books:

1. Physical Chemistry: A Molecular Approach by Donald A. McQuarrie and John D. Simon (University science books)
2. Physical Chemistry by Peter Atkins and Julio de Paula (Oxford)
3. Symmetry and Spectroscopy of molecules, K Veera Reddy, New Age International publishers
4. Principles of fluorescence spectroscopy By Joseph R. Lackowicz (Springer)
5. Modern Spectroscopy, J. M. Hollas, John Wiley, 4th Edn., 2004.
6. Mass Spectrometry: Principles and applications Edmond de Hoffmann and Vincent Stroobant (John Wiley, 3rd edition)