

**JCL 305 (Jan) (3-1-0)****Organic Spectroscopy**

*Instructor: Bani Kanta Sarma*

- Electromagnetic spectrum, various spectroscopic methods, and information they provide. Factors that affect the spectral line width and intensity of lines, concept of selection rule.
- Basic principle of UV-Vis spectroscopy, concept of chromophore, orbitals involved UV-Vis spectroscopy, effect of conjugation on HOMO-LUMO gap, Beer's and Lambert's law, Solvent effect in UV-Vis Spectroscopy, Woodward rules, Isosbestic point and its importance, Applications of UV-Vis spectroscopy with examples.
- Basics of Fluorescence spectroscopy, Jablonski diagram, Phosphorescence, applications of FL with examples.
- Basic principle of CD spectroscopy and its applications, Examples of CD spectra of DNA and various protein secondary structures, differentiating polyproline I and polyproline II helices by CD spectroscopy, DNA and protein (e. g. collagen) melting studies by CD.
- Basics of mass spectrometry, introduction to EI, ESI and MALDI mass spectroscopic methods, concept of molecular ion peak, isotopic pattern, Nitrogen rule, fragmentation pattern, McLafferty rearrangement, fragmentation of peptides by MALDI MS MS.
- Basics of IR spectroscopy, concept degrees of freedom, determining the number of stretching and bending modes in a molecule, various types of vibrational modes, combination bands, overtones and Fermi resonance, hot bands, various functional group analysis by IR, fingerprint region, effect of conjugation, ring strain and hydrogen bonding on IR bands.
- Basic principle of NMR spectroscopy, resonance condition in NMR, NMR active nuclei,  $^1\text{H}$  NMR, chemical shift, splitting and integration in  $^1\text{H}$  NMR, basic idea of  $^{13}\text{C}$  and  $^{19}\text{F}$  NMR. Study of keto-enol tautomerism, intramolecular hydrogen bonding, H/D exchange using NMR spectroscopy. Variable Temperature (V/T) NMR studies. Determining molecular formula from elemental analysis, calculating double bond equivalents (DBE) and structure determination of organic molecules using combination of various spectroscopic methods. Introduction to 2D methods such as NOESY,  $^1\text{H}$ - $^1\text{H}$  COSY, HMBC, HMQC and TOCSY and their analysis for structure determination of complex organic molecules.

**Reference Books:**

1. Organic Spectroscopy by William Kemp
2. Spectroscopic Identification of Organic Compounds by Silverstein