CY51003: Spectroscopic Methods of Structure Determination (**NMR, Mass, IR, UV**).

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Course Outline: *uncorrected and may change depending on the situation.*

What we will learn? (Total available time approx 56 h, **Autumn Semester 2015)**

Entry	Topic /Subject (We will cover in this semester)	Schedule time
A	Determination of molecular structure by utilization of IR Spectra in conjunction with other spectral data: A brief discussion of IR and its applications covering its basic theory **Content:** Introduction: Why we need IR spectroscopy? Basic theory, Hooke's Law, Simple Harmonic Oscillator and Anharmonic Oscillator, characteristic functional groups, ring strain, electronic effect, conjugation effects, concentration effect, etc.	**5 h**
B	Mass Spectroscopy to determine molecular mass. **Content:** Introduction: usefulness of MS (**1 h**). Basic theory, resolution (HRMS and low resolution MS), different ionization technique (CI, EI, ESI, MALDI, FAB) & their application (**4h**), exact mass & isotopic distribution (**3h**), fragmentation & application (4**h**), DBE, etc.	**12 h (3 week)**
C	NMR to determine molecular structure: Majority of our focus will remain on ^{1}D NMR of some important nuclei: **^{1}H, ^{13}C, ^{19}F, ^{31}P,** ^{29}Si, ^{11}B, ^{14}N etc. **Content:** History, basic theory, electromagnetic radiation-and its magnetic component, EPR and its principle similarity with nmr (**1 h**), magnetogyric ratio and its effect (**0.5h**), nmr sensitivity and its magnetic field, temperature & isotopic abundance dependence, why UV and IR are more sensitive technique than NMR? (**1h**), nmr active and inactive nuclei (**1h**), nmr pulses, signal recording (**1h**), nmr instrumentation, FID, Fourier transformation (**1 h**), relaxation (spin-latice and spin-spin), chemical shift, shielding of nucleus, nmr scale, why it is important, δ-value & information extraction, nmr standard peak and solvents (**3 h**), integration and its applications in polymer and simple molecules (**2 h**), coupling constant & multiplicity, satellite peak, specific illustrative	**24 h + 8 h (5 + 2 week)** Tutorial (**rest of the classes**)

	examples and cases (**4 h**), molecular anisotropy, nmr time scale and its application in conformational analysis, trapping of conformation at lower temp., determination of enantiomeric ratio (**1 h**), ^{31}P and ^{19}F NMR and application (**1h**), 2D NMR and its application (**3 h**), **Problem solving:** NMR of simple to more complex structure (**5 h** and rest of the time), organometallic complexes (**2 h**), protein in folded and unfolded conformation (**1 h**)	

References:

For IR and Mass: Books

1. Spectroscopic Identification of Organic Compounds
   Authors: Silverstein, R. M. and Wenster, F. X.
2. Fundamental of Molecular Spectroscopy
   Authors: Banwell, Colin. N. and McCash, Elaine M.
3. Any other Basic book of your choice.

NMR: Books

1. NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry
   Author: Harald Gunther
2. Basic One- and Two Dimensional NMR Spectroscopy
   Author: Horst Friebolin
3. Title: Spectroscopic Identification of Organic Compounds
   Authors: Silverstein, R. M. And Wenster, F. X.
4. Any basic books on NMR Spectroscopy of your choice.