Course No.	Course Name	L-T-P-Credits
CY 408	**Molecular Spectroscopy**	**3-0-0: 03**
Prerequisite: NIL		

Course Objectives: The main objective of the course is to provide basic knowledges of molecular spectroscopy. The course is planned to present to the students the physical aspects of various spectroscopy. The course is relevant to interpret phenomenon of the interaction of light with matter in terms of the relationship with the molecular structure. The course will be useful for the students in the understanding molecular properties and spectra.

Course Outcomes: After successful completion of the course, students will be able to:

1. Identify the terms in and describe various laws of molecular spectroscopy.
2. Explain why atomic spectra consist of lines whereas molecular spectra at room temperature are broad and continuous.
3. Describe the effect of changing the slit width and the impact it will have on qualitative and quantitative analyses.
4. Outline the selection rules for different spectroscopy and indicate the involvement of molecular dipole moment for the analysis of selection rules.
5. Determine the vibrations for a triatomic molecule and identify whether they are infrared-active.
6. Explain the difference between Stokes and anti-Stokes lines in a Raman spectrum.
7. Draw an energy level diagram and identify the transitions that correspond to absorption, fluorescence, internal conversion, radiation-less decay, intersystem crossing and phosphorescence.
8. Explain the difference between a three and four level laser.

SYLLABUS

Module	Contents	Hours
I	**Introduction** Electromagnetic radiation, interaction of electromagnetic radiation with matter, natural line width and natural line broadening, intensity of spectral lines, time dependent perturbation theory, semi-classical treatment, derivation of probability of spectral transition-concept of absorption and emission, derivation of selection rules, Born-Oppenheimer approximation.	06
II	**Rotational and vibrational Spectroscopy** Classification of molecules according to their moments of inertia, rotational energy levels, selection rule, intensity of spectral lines, effect of substitution in microwave spectra, stark effect, spectra of symmetric top and asymmetric top type molecules. Linear harmonic oscillator, vibrational energy levels of diatomic molecules, anharmonicity, potential energy diagram, vibration–rotational spectra of diatomic molecules, polyatomic molecules (CO_2, NH_3 etc.) selection rules, fundamental, overtone and combination bands, hot bands, group frequencies, factors affecting the band positions and intensities, far I.R. regions, brief description of instrumental techniques. Theories of Raman Effect, condition for Raman active vibrations, selection rules, mutual exclusion	15

	principle, rotational Raman spectra, vibration–rotation Raman spectra.	
III	**Electronic Spectroscopy** Born-Oppenheimer approximation, Frank-Condon principle, ground and excited states of diatomic molecules, selection rules for electronic transitions; Fluorescence, phosphorescence and Chemiluminescence; Optical rotatory dispersion and circular dichroism (ORD and CD) spectroscopy, electronic spectra of polyatomic molecule, Beer-Lambert's law, chromophores, auxochromes, solvent effect, calculation of absorption maxima by Woodward-Fieser Rules.	07
IV	**Mössbauer spectroscopy** Nuclear resonance absorption, recoil energy, Doppler Effect, Mössbauer effect, isomer shifts, quadrupole splitting, effect of magnetic field, applications to iron, tin and cobalt compounds.	03
V	**Time Resolved Spectroscopy** Introduction, phenomenon associated with non-linear optics (NLO), two photon absorption, principle of laser (two, three and four level laser systems), and time resolved spectroscopy, applications to chemical and biological problems.	05

Essential Readings:

1. C. N. Banwell and E. M. McCash, "Fundamentals of Molecular Spectroscopy", Tata McGraw Hills, 4th Edition, 2017.
2. P. Atkins and J. D. Paula, "Atkins' Physical Chemistry", Oxford University Press, 11th Edition, 2018.

Supplementary Readings:

1. D. N. Sathyanarayana, Handbooks of Molecular Spectroscopy, IK International Publishing House, 2nd Edition, 2019.
2. P. S. Sindhu, "Fundamental of Molecular Spectroscopy", New Age publishers, 2nd Edition, 2011.
3. B. B. Laud, "Laser and Non Linear Optics", New-Age-International Publisher, 3rd Edition, 2011.
4. I. N. Levine, Molecular Spectroscopy, Wiley-Blackwell, 1st Edition, 1975.