Curriculum Plan (Odd Semester 2022-23)

Teacher Name: **Dr. Sajid Iqbal**
Course: B.Sc. (H) Chemistry, CBCS, Sem V
Paper Name: Physical Chemistry V (CBCS): Quantum Chemistry & Spectroscopy (4 periods per week)
UPC: 32171502

S.No.	Contents	Allocation of Lectures	Monthwise schedule to be followed	Assignments/ Presentations etc
1.	**Quantum Chemistry:** Postulates of quantum mechanics, quantum mechanical operators and commutation rules, Schrödinger equation and its application to free particle and particle-in-a box (rigorous treatment), quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle; wave functions, probability distribution functions, nodal properties, Extension to two and three dimensional boxes, separation of variables, degeneracy	16	20th July-2nd week of August	• Overview of Syllabus • Numerical Problem Solving • Doubt Session
2.	Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wave functions. Vibrational energy of diatomic molecules and zero-point energy	4	3rd week of August – 1st week of September	• Numerical Problem Solving • Doubt Session
3.	Angular momentum. Rigid rotator model of rotation of diatomic molecule. Schrödinger equation in Cartesian and spherical polar. Separation of variables. Spherical harmonics. Discussion of solution (Qualitative).	4	1st week of September – 2nd week of September	• Numerical Problem Solving • Doubt Session • Assignment Distribution
4.	Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus. Setting up of Schrödinger equation for many-electron atoms (He, Li). Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).	4	3rd week of September - 4th week of September	• Numerical Problem Solving • Doubt Session • Class Test • University Papers Discussion
5.	**Molecular Spectroscopy:** Interaction of electromagnetic radiation with molecules and various types of spectra; Born Oppenheimer approximation. **Rotation spectroscopy:** Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.	12	1st week of October-3rd week of October	• Numerical Problem Solving • Doubt Session • Assignment Collection

	Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, overtones, hot bands, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.			
6.	**Raman spectroscopy:** Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion. **Electronic spectroscopy:** Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model.	4	4th week of October	• Numerical Problem Solving • Doubt Session • Class Test
7.	**Nuclear Magnetic Resonance (NMR) spectroscopy:** Nuclear Magnetic Resonance (NMR) spectroscopy: Principles of NMR spectroscopy, Larmor precession, chemical shift and low resolution spectra, different scales (δ and T), spin-spin coupling and high resolution spectra, interpretation of PMR spectra of simple organic molecules like methanol, ethanol, acetaldehyde, acetic acid and aromatic proton.	12	1st week of November -15th November	• Numerical Problem Solving • Doubt Session • Previous Year Paper and Expected Question Discussion