Curriculum Plan (Odd Semester 2024-25)

Teacher Name: **Dr. Sajid Iqbal**
Course: B.Sc. (H) Chemistry, UGCF-NEP-2020, Sem V
Paper Name: DSC15: Quantum Chemistry & Covalent Bonding (3 periods per week)

S. No.	Contents	Allocation of Lectures	Month wise 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.	12	1st August -1st week of September	• 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	5	2nd week of September – 4th week of September	• Numerical Problem Solving • Doubt Session • Class Test
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).	5	1st week of October – 2nd week of October	• Numerical Problem Solving • Doubt Session • Assignment Distribution
4.	**Hydrogen atom** Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part and quantization of energy (only final energy expression). Average and most probable distances of electron from nucleus. Zeeman effect, Introduction of spin quantum number and magnetic spin quantum number Setting up of Schrödinger equation for many electron atoms (He, Li), Indistinguishability of electrons and Pauli exclusion principle, Need for approximation methods. Statement of variation theorem and application to simple systems (particle-in-a-box, harmonic oscillator, hydrogen atom).	8	3rd week of October – 1st week of November	• Numerical Problem Solving • Doubt Session • Class Test
5.	**Covalent Bonding** Setting up of Schrödinger equation, Born-Openheimer approximation, LCAO-MO treatment of H_2^+ and its qualitative extension to H_2, Valence bond (VB) treatment of H_2, Comparison of LCAO-MO and VB wave functions of H_2 and their refinements, Qualitative description of LCAO-MO of homonuclear and heteronuclear diatomic molecules-HF and LiH.	15	1st week of November – 24th of November	• Doubt Session • Class Test • University Papers Discussion