

CURRICULUM PLAN, Even Semester 2021

Dr. Upasana Issar

B.Sc. (H) Generic Elective, II Year (Semester IV)

Name of Paper: Ge5: Chemistry of d-Block Elements, Quantum Chemistry & Spectroscopy (CBCS)

UPC: 32175916

Section B: Physical Chemistry-4

Contents	Allocation of Lectures	Month wise schedule to be followed	Tutorial/Assignments/Presentation etc
<p>Quantum Chemistry</p> <ul style="list-style-type: none"> • Postulates of quantum mechanics, quantum mechanical operators. • Free particle. • Particle in a 1-D box (complete solution), quantization, normalization of wavefunctions, concept of zero-point energy. • Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results (solution not required). Quantization of vibrational energy levels. 	09	1 st week of Jan- 1 st week of Feb	Numerical Solving Doubt Session
<p>Quantum Chemistry (Contd.) <i>Rotational Motion:</i> Schrödinger equation of a rigid rotator and brief discussion of its results (solution not required). Quantization of rotational energy levels.</p> <p>Spectroscopy</p> <ul style="list-style-type: none"> • Spectroscopy and its importance in chemistry. • Wave-particle duality. • Link between spectroscopy and quantum chemistry. 	08	1 st week of Feb- 4 th week of Feb	Numerical Solving Doubt Session Assignment Distribution

<ul style="list-style-type: none"> • Electromagnetic radiation and its interaction with matter. Types of spectroscopy. Difference between atomic and molecular spectra. • Born- Oppenheimer approximation: Separation of molecular energies into translational, rotational, vibrational and electronic components. 			
<p>Microwave (pure rotational) spectra of diatomic molecules. Selection rules. Structural information derived from rotational spectroscopy.</p> <p>Vibrational Spectroscopy: Selection rules, IR spectra of diatomic molecules. Structural information derived from vibrational spectra. Vibrations of polyatomic molecules. Group frequencies. Effect of hydrogen bonding (inter- and intramolecular) and substitution on vibrational frequencies.</p> <p>Electronic Spectroscopy: Electronic excited states. Free Electron model and its application to electronic spectra of polyenes. Colour and constitution, chromophores, auxochromes, bathochromic and hypsochromic shifts.</p>	07	1 st week of March- 3 rd week of March	Numerical Solving Doubt Session
<p>Photochemistry</p> <ul style="list-style-type: none"> • Laws of photochemistry. • Lambert Beer's law. • Fluorescence and phosphorescence. • Quantum efficiency and reasons for high and low quantum yields. • Primary and secondary processes in photochemical reactions. Photochemical and thermal reactions. • Photoelectric cells. 	08	1 st week of April – 4 th week of April	Numerical Solving Doubt Session University Papers Discussion