Name: **Enrolment No:**	

UPES

End Semester Examination, May 2024

Course: Advanced Physical Chemistry **Semester: VI**

Program: Int. B.Sc. M.Sc. Chemistry **Time: 03 hrs.**

Course Code: CHEM3026 **Max. Marks: 100**

Instructions:

- Write your name and enrolment no. at the top of the question paper.
- Do not write anything else on the question paper except your name and roll number.
- Attempt all the parts of a question at one place only.
- CO1, CO2, CO3 & CO4 in the last column stand for course outcomes and are for official use only.

SECTION A
(5Qx4M=20Marks)

S. No.		Marks	CO
Q 1	What are the gross selection rules of rotational, vibrational, and Raman spectroscopy?	**4**	**CO1**
Q 2	What are the properties of a wavefunction? Not every function can be a wavefunction.	**4**	**CO2**
Q 3	Given a classical observable (position, momentum, kinetic energy, total energy), write down the corresponding quantum operators.	**4**	**CO1**
Q 4	The percent transmittance of 10^{-4} M solution of malachite green is 40 when measured at 620 nm in a cell of pathlength of 1 cm. Calculate the absorbance and molar extinction co-efficient.	**4**	**CO3**
Q 5	What is radial probability density function? Draw radial probability distribution curve for 1s, 2s and 2p orbital of H atom.	**4**	**CO1**
	SECTION B **(4Qx10M= 40 Marks)**		
Q 6	(a) Plot $\psi_n(x)$ and $\psi_n^2(x)$ for a particle in a box (with infinite height walls) with n=1,2,3,4 for 0<x<L. (b) Write the Schrödinger equation and energy expression of harmonic oscillator.	**5+5**	**CO3**
Q 7	(a) Calculate the average momentum of a particle in vibrational state "v" which is described by wave function "ψ_v" (b) The energy of 1st excited state of 1D SHO is 400 cm^{-1}; what is the energy of the next higher energy level?	**5+5**	**CO2**
Q 8	(a) Discuss the classical mechanical picture of light-matter interaction phenomena.	**5+5**	**CO2**

	(b) Give the quantum mechanical expression of energy of a rigid rotor. If B = 25 cm^{-1} give the rotational energy levels of this molecules J= 0, 1,2,3.		
Q 9	List the postulates of quantum mechanics and explain them. **OR** The vibration of $^{1}H^{35}Cl$ molecule can be considered as simple harmonic oscillation. The force constant is 400 Nm^{-1}. Calculate the fundamental vibration frequency and 1st excited vibrational energy of this molecule in joules. (Given: Plank constant = 6.626×10^{-34} Js).	**10**	**CO3**
SECTION-C (2Qx20M=40 Marks)			
Q 10	(a) Show that the wavefunction $\psi(x)=Ne^{ik}$ of the free particle is an eigenfunction of the linear momentum operator $\hat{p}$. Find the average linear momentum for a particle in state $\psi(x) = Ne^{ikx}$. (b) (i) Draw an energy diagram indicating the origin of fundamental, first overtone, 2nd overtone and hot band in vibrational spectroscopy. (ii) Show the origin of the P, Q, and R branches in rovibrational spectroscopy.	**10+10**	**CO2**
Q 11	(a) Derive thermodynamic master equations and criteria of spontaneity from thermodynamic square. (b) Explain the distinctions between Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac statistics. **OR** (a) Explain one of the approximate theories in quantum mechanics, either (i) perturbation theory or (ii) variation theorem. (b) Discuss the principles of Debye-Huckel Theory.	**10+10**	**CO4**