Name:

Enrolment No:

UPES

End Semester Examination, December 2023

Course: Quantum Chemistry **Semester: I**

Programme: MSc (Chemistry) **Time: 03 hrs**

Course Code: CHEM 7047 **Max. Marks: 100**

Nos. of page(s): 3

Instructions: Read all the below mentioned instructions carefully and follow them strictly

1) Write your name and enrollment no. at the top of the question paper.
2) Do not write anything else on the question paper except your name and roll number.
3) Attempt all the parts of a question at one place only.
4) Internal choices are given for question number 9 and 11.
5) CO1, CO2, CO3 & CO4 in the last column stand for course outcomes and are for official use only.

SECTION A

(Attempt all Five Questions) (5Qx4M=20Marks)

S. No.		Marks	CO
Q 1	Draw the potential energy diagram of a simple harmonic oscillator and draw the graph of ψ^2 vs r plot where ψ is the vibrational wavefunction. Indicate the Energy of each vibrational state.	**4**	**CO1**
Q 2	Calculate the eigen value of a function $\psi = 4e^{-6x}$ when the operator is $\frac{d^2}{dx^2}$.	**4**	**CO3**
Q 3	Write the Schrodinger equation of a hydrogen atom in polar and Cartesian co-ordinate.	**4**	**CO1**
Q 4	Which orbital has two radial and two angular nodes?	**4**	**CO2**
Q 5	(i) Write the Schrodinger equation of a particle in three-dimensional box. (ii) What is the energy expression of a particle in a cubic box.	**4**	**CO3**

SECTION B

(Attempt all Questions; internal choice is given for question number 9) (4Qx10M= 40 Marks)

Q 6	**(a)** Assume hexatriene as particle in one dimensional box with L= 0.85 nm. What is the wavelength (nm) of light required for the transition from ground state to the first excited state? **(b)** A particle in 3D cubic box of length "a" has energy of $\frac{14h^2}{8ma^2}$. What is the degeneracy of the state?	**6+4**	**CO2**
Q 7	(a) What is the expression of rotation constant **B** (cm^{-1}) in terms of moment of	**5+5**	**CO2**

	inertia? If B = 20 cm^{-1}, what are the energies of the rotational energy levels of the molecule with J= 0, 1, 2 and 3? (b) Write the Schrodinger equation of a simple harmonic oscillator. What is zero-point energy?		
Q 8	**(a)** The rotation of HF can be modelled as rigid rotor. The energy difference between the 4^{th} and 5^{th} rotational level is 200×10^{-23} J. Calculate the energy of the rotational level with J=1. **(b)** Draw the radial probability density plot of 1s, 2s, and 2p orbitals.	**10**	**CO2**
Q 9	**(a)** The vibration of $^{35}Cl^{35}Cl$ molecule can be considered as simple harmonic oscillation. The force constant is 240 Nm^{-1}. Calculate the fundamental vibration frequency and the zero-point energy of this molecule. **OR** Calculate the average momentum of a particle in vibrational state "v" which is described by wave function "ψ_v". Justify your answer. **(b)** Find the value of the commutator [x, p_x] and [p_x, T_x] where p_x, T_x are momentum and kinetic energy operators along the X direction. **OR** What is Hermitian operator? Prove that the Hermitian operators always give real eigen value.	**5+5**	**CO3**
SECTION-C (**Attempt all Questions; internal choice is given for question number 11**) **(2Qx20M=40 Marks)**			
Q10	**(a)** Derive the expression of wave function and energy of a particle in three-dimensional box. **(a)** (i) Draw the wavefunction and energy levels of a simple harmonic oscillator. (ii) The lowest energy of 1D SHO is 300 cm^{-1}, What is the energy of the next higher energy level?	**10+10**	**CO4**
Q 11	**(a)** (i) Derive the expression of angular momentum operators along X, Y and Z directions. (ii) What is the value of the commutator [L^2, L]? **OR** Given that a particle is restricted to the region –a<x<a and has a wave function ψ proportional to $\mathbf{cos}\left(\frac{\pi x}{2a}\right)$, normalize the wave function. **(b)** Calculate the force constant of the molecule ($^1H^{35}Cl$) if the separation of its	**10+10**	**CO4**

	two lowest vibrational energy level is 3.313×10^{-20} J. **OR** Which of the following functions are acceptable as wave functions? Explain (i) $\psi = e^{2x}$ (ii) $\psi = e^{-x}$ (iii) $\psi = e^{-x^2}$ (iv) $\psi = \sin x$ (v) $\psi = \tan x$		