Name: **Enrolment No:**	UPES UNIVERSITY OF TOMORROW

UPES

End Semester Examination, December 2023

Course: Physical Chemistry V **Semester: V**

Program: B.Sc. (H) Chemistry **Time : 03 hrs.**

Course Code: CHEM 3015 **Max. Marks: 100**

Instructions: Read the instructions given below carefully:

1. **All questions are compulsory.**
2. **Internal choice is given in Q 9 and 11.**

SECTION A
(5Qx4M=20Marks)

S. No.		Marks	CO
Q 1	Calculate the speed of an electron if its de Broglie wavelength is 0.1 nm. (m_e= 9.1 x 10^{-31} Kg; h=6.6 x 10^{-34} Js)	**4**	**CO1**
Q 2	What is the selection rule for a vibrational and pure rotational spectrum?	**4**	**CO3**
Q 3	In proton NMR spectra determination, how many kinds of proton are there in the following compounds: **a)** $CH_3CH_2CH_3$ **b)** $(CH_3)_2CHCH_2CH_3$	**4**	**CO2**
Q 4	Evaluate the commutator [$\varkappa$, d/d$\varkappa$] operating on an arbitrary function f($\varkappa$).	**4**	**CO1**
Q 5	Write down the values of Laplacian and Hamiltonian operators?	**4**	**CO1**
	SECTION B **(4Qx10M= 40 Marks)**		
Q 6	Calculate the expectation value of distance $\langle x^2 \rangle$ for a particle in a one-dimensional box in between 0 to a; given that the normalized wave function is $\Psi = \frac{\sqrt{2}}{a} \sin \frac{n\pi\varkappa}{a}$	**10**	**CO2**
Q 7	What are the main points of similarities and differences between VBT and MOT?	**10**	**CO2**
Q 8	Derive the Schrodinger wave equation for a particle moving in a 3-dimensional box.	**10**	**CO1**
Q 9	What is Infrared spectroscopy. Discuss the various modes of vibrations and regions found in IR spectra with total energy expression of the molecule.	**10**	**CO3**

	OR With the help of a schematic diagram, explain briefly the Shielding and Deshielding of Protons in NMR studies.		
SECTION-C (2Qx20M=40 Marks)			
Q 10	**(a)** Calculate wavelength of an electron having kinetic energy equal to 4.55×10^{-25}J. ($m_e = 9.1 \times 10^{-31}$ Kg; h=6.6×10^{-34} Js) **(b)** According to Born Oppenheimer approximation, what is the value of electronic Hamiltonian for a diatomic molecule like H_2? Discuss in detail.	**10** **10**	**CO2**
Q 11	**a)** Discuss Franck-Condon principle in vibrational spectrum. With the help of a suitable diagram, discuss all possible electronic transitions with localized molecular orbitals in a carbonyl group. **OR** Calculate the vibrational frequency of CO in cm^{-1} if its force constant is 1840 Nm^{-1}. The atomic masses are $^{12}C = 19.9 \times 10^{-27}$ kg and $^{16}O = 26.6 \times 10^{-27}$ kg. **b)** A sample was excited by the 435.8 nm line of mercury. A Raman line was observed at 4447 A^0. Calculate the Raman shift in cm^{-1}. At what wavelength in A^0 would the anti-stokes line appear in the Raman spectrum of the sample. **OR** The pure rotational spectrum of gaseous HCl contains a series of equally spaced lines separated by 20.80 cm^{-1}. Calculate the internuclear distance of the molecule. The atomic masses of H and Cl are 1.673×10^{-27} kg and 58.06×10^{-27} kg respectively.	**10** **10**	**CO3**