**Name:**

**Enrolment No:**

**UNIVERSITY OF PETROLEUM AND ENERGY STUDIES**
**End Semester Examination, December 2022**

**Course: Physical Chemistry V** **Semester: V**
**Program: B.Sc. (Hons.) Chemistry** **Duration: 03 hrs.**
**Course Code: CHEM 3002** **Max. Marks: 100**

**Instructions: Read the instructions given below carefully:**

1. **All questions are compulsory.**
2. **Internal choice is given in question 4 of Section B and question 2 of section C.**

**SECTION A**
**(5Qx4M=20Marks)**

| S. No. | | Marks | CO |
|---|---|---|---|
| **Q 1** | Calculate the uncertainty in the velocity of an electron if the uncertainty in its position is approximately 1 Å. | **4** | **CO1** |
| **Q 2** | Explain the terms: Red shift, Blue shift, Hyperchromic and Hypochromic shift. | **4** | **CO3** |
| **Q 3** | List out the different modes of vibrations found in an IR spectroscopy. | **4** | **CO2** |
| **Q 4** | An electron in a one-dimensional box of width 2 Å undergoes transition from the ground state to the first exited state. Calculate the transition energy in eV. ($m_e$= 9.1 x $10^{-31}$ Kg. | **4** | **CO1** |
| **Q 5** | Discuss the conditions of normalized and orthogonal wave functions. | **4** | **CO1** |

**SECTION B**
**(4Qx10M= 40 Marks)**

| | | | |
|---|---|---|---|
| **Q 1** | Using the normalized wave function, $\Psi 1s = \frac{1}{\sqrt{\pi} a_o^{3/2}} e^{-r/a_o}$, for the ground state of hydrogen atom, calculate the probability for the electron to be confined in a sphere of radius r = $a_0$, the Bohr radius. | **10** | **CO2** |
| **Q 2** | Discuss how the wave function of a diatomic molecule like $H_2$ has been explained according to VBT? | **10** | **CO2** |
| **Q 3** | Derive an expression for the energy of a rigid rotator using the Schrodinger wave equation.. | **10** | **CO1** |
| **Q 4** | List all the electronic transitions possible for<br>**a)** $CH_3CH_2CH_3$<br>**b)** $CH_3CH_2Cl$ | **10** | **CO3** |

| | | | |
|---|---|---|---|
| | **c)** $CH_3(C{=}O)H$<br><br>**OR**<br><br>Illustrate the Frank-Condon principle in the vibrational spectrum of a diatomic molecule with suitable potential energy curve. Show diagrammatically all possible electronic transitions with localized molecular orbitals for the carbonyl group. | | |
| **SECTION-C**<br>**(2Qx20M=40 Marks)** | | | |
| **Q 1** | **(a)** Write all possible energy levels below $16h^2/8ma^2$ for a particle moving in a 3-dimensional box having edge length a=b=c. Illustrate them with the help of energy profile diagram.<br>**(b)** Apply quantum mechanical principles to calculate the coefficients of atomic orbitals in $sp^3$ hybrid orbitals and write their wave functions. | **20** | **CO2** |
| **Q 2** | **(a)** Draw the energy level diagram and the spectral transitions for the microwave (pure rotational) spectrum of a rigid diatomic rotator using the energy level expression and the selection rules. Also derive the expression for wavenumber (in $cm^{-1}$) for P-Branch of spectra.<br><br>**OR**<br><br>With the help of a schematic diagram, explain briefly the Shielding and Deshielding of Protons in NMR studies.<br><br>**(b)** If $H^{35}Cl$ is irradiated with 435.8 nm mercury line, calculate the Raman line in nm if the fundamental vibrational frequency of $H^{35}Cl$ is $8.667 \times 10^{13}$ $s^{-1}$.<br>**OR**<br>The internuclear distance of CO molecule is 1.13 Å. Calculate the energy (in joules and in eV) of this molecule in the first excited rotational energy level. The atomic masses are: 12C = $1.99 \times 10^{-26}$ kg and 16O = $2.66 \times 10^{-26}$ kg. | **20** | **CO3** |