CML101: Tutorial 4 - Quantum Chemistry
UG Semester - I (2023-24)

Q1: The ground-state wave function of a quantum harmonic oscillator is given as,

$$\psi_0(x) = \left(\frac{b}{\pi}\right)^{1/4} e^{-bx^2/2}$$

Show that $\Delta p_x \Delta x = \frac{\hbar}{2}$. Where $\Delta p_x = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2}$ and $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ are the variances in p_x and x, respectively.

Q2: A strong absorption band of infrared radiation is observed for $^1H^{35}Cl$ at 2991 cm^{-1}. (a) Calculate the force constant, k, for this molecule. (b) By what factor do you expect the frequency to shift if H is replaced by D? Assume that the force constant does not get affected by this change.

Q3: Derive the expression for the standard deviation of the bond length of a diatomic molecule when it is in its ground state. (b) What percentage of the equilibrium bond length is this standard deviation for CO in its ground state? For CO, $\tilde{\nu} = 2170$ cm^{-1} and Re = 113 pm.

Q4: The wave function of the ground state of H atom is given as, $\psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$.

(i) Find the average distance of 1s electron from the nucleus in the hydrogen atom.

(ii) Calculate the most probable distance (i.e., radius) at which the 1s electron of H-like atom with atomic number Z is to be found. Show that as Z increases, this most probable distance decreases.

Q5: Calculate the ground state energy of the hydrogen atom in SI units and convert the result to electronvolts (eV).

$$E_n = -\frac{Z^2}{n^2} \frac{e^2}{8\pi\epsilon_0 a} = \frac{Z^2 \mu e^4}{8\epsilon_0^2 n^2 h^2} \tag{1}$$

where $a = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2}$

[Given $m_e = 9.109 \times 10^-31$ kg, $e = 1.602 \times 10^-19$ C, $\epsilon_0 = 8.854 \times 10^{-12}$ $C^2/N\text{-}m^2$, 1 eV = 1.602 $\times 10^{-19}$ J]

Q6: Calculate the wavelength and frequency for the spectral line that axis from n=5 to n=3 transition in the H-atom. [Rydberg constant (R_H) = 1.097373 $\times 10^7 m^{-1}$ and c=3×10^8 m/s]