CHM 330 - Worksheet 4 Prof. Andrew J. Pounds Spring 2022

Name_____

- 1. Using the particle in a 1-D box model with infinitely high potential walls, calculate the **wavelength** of the photon, in nm, that is emitted when an electron goes from the LUMO to the HOMO in 1,3,5,7,9-decapentaene. You may assume that C-C single bonds have a length of 154 pm and C=C double bonds have length of 135 pm. (20 pts)
- 2. For a particle trapped in the first eigenstate of the 1D particle in an box with infinitely high potential walls, the normalized eigenfunction is

$$\psi(x) = \begin{cases} \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin\left(\frac{\pi x}{L}\right) & 0 \le x \le L \\ 0 & \text{othewise} \end{cases}$$

What is the **probability** of finding the particle between $\frac{L}{4}$ and $\frac{3L}{4}$? (20 pts)

3. Suppose a particle in a 1D box is in a state represented by the normalized eigenfunction

$$\psi(x) = \begin{cases} \left(\frac{30}{L^5}\right)^{\frac{1}{2}} x \left(L - x\right) & 0 \le x \le L \\ 0 & \text{othewise} \end{cases}$$

What is the **expectation value** of the **total energy** for this eigenstate? (20 pts)

- 4. The infrared spectrum of ${}^{75}\text{Br}{}^{19}\text{F}$ consists of an intense band (which is $\bar{\nu}_0$) at 380 cm⁻¹. What is the value of the **force constant**, k, in N·m⁻¹ for ${}^{75}\text{Br}{}^{19}\text{F}$. (20 pts)
- 5. It takes photons with a maximum wavelength of 564 nm to eject electrons from potassium metal. What is the velocity (in $m \cdot s^{-1}$) of electrons ejected from potassium metal if the **incident** radiation has a wavelength of 410 nm. (20 pts.)
- 6. For the following two angular wavefunctions $(Y_l^{m_l})$, demonstrate that they are normalized and orthogonal.

$$Y_1^0(\theta,\phi) = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}}\cos\left(\theta\right)$$

$$Y_2^1(\theta,\phi) = \left(\frac{15}{8\pi}\right)^{\frac{1}{2}} \sin\left(\theta\right) \cos\left(\theta\right) \cos\left(\phi\right)$$

Section_____