Quantum Mechanics and Spectroscopy
CHEM 3PA3
Assignment 12 **Name:** _____

1. Consider the following hydrogen wavefunction.

$$\psi_{3p_0}(\mathbf{r}) = \sqrt{\frac{2}{3^8\pi}} \cdot (r)(6-r)e^{-r/3}\cos\theta$$

   (a) Find the roots, maximum and minimum points of the radial wavefunction.

   (b) Obtain the expression for the radial probability distribution,

$$P(r) = \int_0^{\pi} \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi \left[|\psi(r,\theta,\phi)|^2 r^2 \sin\theta \right].$$

   (c) Find the roots, maximum and minimum points of the probability distribution.

   (d) Draw a rough sketch of the radial wavefunction and the probability distribution.

   (e) Draw a rough sketch of the angular part of the wavefunction.

2. Consider the following operators:

$$\hat{L}_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$
$$\hat{L}_y = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$
$$\hat{L}_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$
$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

   Which of the pairs of operators commute?

3. A parameter, ζ, was introduced to minimize the energy of the 2-electron ground-state atom, The expression for the energy is:

$$E(\zeta) = -\zeta^2 + \frac{5}{8}\zeta + 2\zeta^2 - 2\zeta Z.$$

   Find the effective nuclear charge that yields the minimum energy and calculate the energy for He.

4. The transition of an electron of the 1-electron atom from energy level n_i to n_f involves the absorption ($n_i < n_f$) or emission ($n_i > n_f$) of a photon. The Rydberg formula relates the wavelength of the photon with the difference in energies of the transition,

$$\frac{1}{\lambda_{vac}} = RZ^2\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right),$$

   where R is $1.09737 \cdot 10^7$ m^{-1}. Derive this equation from the energy expression of the 1-electron atom. Substitution of n_i and n_f directly in the formula when $n_i > n_f$ yields a negative wavelength, is this possible?