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

1. Write the electronic Hamiltonian of a Li atom and indicate the interaction that each term corresponds to. Write its Slater determinant.

2. Consider an electron in a two-dimensional box of dimensions a, and b,

$$\Psi_{n_x,n_y}(x,y) = \left(\frac{4}{ab}\right)^{1/2} \sin\frac{n_x\pi x}{a} \sin\frac{n_y\pi y}{b}$$

   (a) Is the wavefunction normalized?

   (b) What is the probability of finding the electron in the ground state inside of the box given by $0 \leq x \leq a/2$, and $0 \leq y \leq b/2$?

   (c) Can you obtain this answer without integration?

   (d) Is there degeneracy for the excited state with lowest energy? If so, when?

3. Consider a 3D particle in a box with dimensions of $5\mathring{A} \times 5\mathring{A} \times 50\mathring{A}$, and make a table of energies with different values for n_x, n_y, and n_z. Make another table to show the first few transitions and the wavelength associated to each of them. Compare it to the wavelengths of transitions for a 1D box of $50\mathring{A}$ of length. Are the values similar? What can you infer about their spectrum?

4. Find the position of the nodes in the wavefunction $n = 4$ for a particle in a 1D box.

   Two operators $\hat{A}$ and $\hat{B}$ commute if $\left[\hat{A},\hat{B}\right]\Psi(x) = \hat{A}\hat{B}\Psi(x) - \hat{B}\hat{A}\Psi(x) = 0$. Do $\hat{l}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$ and $\hat{l}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$ commute?