CHEM442-001/002 Name ______________________________
College of Charleston
Spring 2001
Exam II Score ___________ /100

1(10). For polyelectronic atoms, four quantum numbers are used to describe the electrons. Identify these by giving the respective name (correct spelling), symbol, and permitted values.

2(10). For atomic Be ($Z = 4$) write the hamiltonian operator (write out all terms) describing the electronic motion.

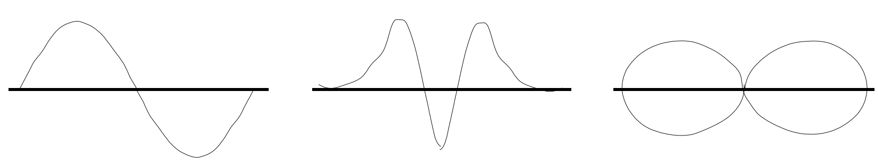
If a trial wave function ϕ for Be is to be constructed using various hydrogen atomic wave functions ψ_{1s}, ψ_{2s}, ψ_{2p}, etc., write the Slater determinant for the ground state of Be. (Do not expand the determinant.)

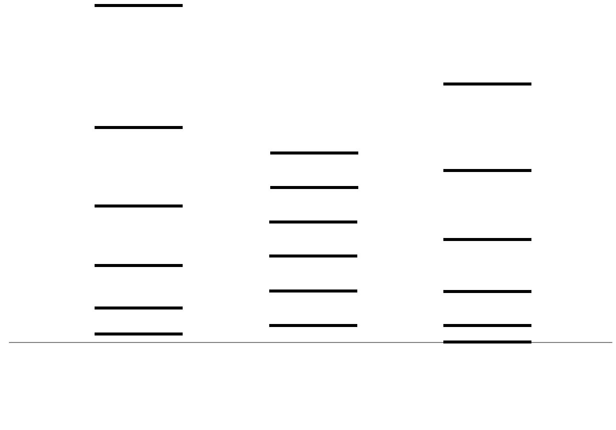
3(10). Write the complete electronic configuration (using the usual subshell notation) for atomic Br ($Z = 35$).

Predict the oxidation number(s) of Br.

What are the four quantum numbers of the 35^{th} electron?

4(15). The following sketches are plots of ψ for a particle in a 1-D box with $n = 2$, a rigid rotator with $J = 2$ and $m = 0$, and a SHO with $v = 2$. Clearly identify each ψ plot. Also shown are plots of energy levels for 1-D box, rigid rotator, and SHO (not to the same scale). Clearly identify each E plot. (Note, the sets of ψ and E plots are not necessarily in the same order.)





5(15). Assume that a nitrogen molecule (atomic mass 14.0) acts as a particle in a 3-D box with $a = b = c = 1.00$ m. Also assume $n_x = n_y = n_z$ (which is quite reasonable). Calculate the value of n_x represented by the thermal energy of $(3/2)k_B T$ at 25 ºC.

6(15). The moment of inertia of a HI molecule is 4.330×10^{-47} kg m^2. Calculate the ratio of the number of molecules with rotational quantum number $J = 2$ to those with $J = 0$ at 25 ºC.

7(25). Determine $\psi_{J,m}(\theta,\phi)$ for a rigid rotator with $J = 2$ and $m = 2$.