Problem Set 5
CHM102A

1. (a) Which orbital of Be^{3+} has the same energy as the 2s orbital of the hydrogen atom?

   (b) The values of shielding constant σ for Li atom are 0.31 and 1.72 for the 1s and 2s orbitals respectively. Calculate the difference in energies between the 1s and 2s orbitals.

2. The first two ionization energies of He-atom are 2372.3 KJ/mol and 5250.4 KJ/mol. Assuming that the electron-electron repulsion in the He-atom can be neglected, calculate the effective nuclear charge of He-atom. What is the total multi-electron wavefunction of the ground state of the He-atom in this approximation (no need to normalize the wavefunction)? Include both the spatial and spin parts.

3. The atomic orbitals of Li have energies $E_{1s} \approx -2.5$ and $E_{2s} \approx -0.2$ Hartrees (where, 1 Hartree = 27.2 eV). Based on energetic criteria alone, qualitatively write down the occupied molecular orbitals of LiH. Given that LiH is ionic *i.e.*, $Li^{+}H^{-}$, what can you say about the atomic orbital coefficients of the highest occupied molecular orbital?

4. As a part of Molecular Orbital Theory that you are studying, a useful, but qualitative concept is that of Bond Order (BO), which is given by:

   BO = ½ |(Number of bonding — Number of antibonding)|

   What is the write the electronic configuration and bond order of the following species: O_2^{-}, N_2^{2+}, F_2. Identify the HOMO and LUMO in the following species: O_2, N_2^{2-}, F_2.

5. The wavenumber of the $j = 1 \leftarrow j = 0$ rotational transitions for $^{1}H^{35}Cl$ and $^{2}H^{35}Cl$ are 20.8784 and 10.7840 cm^{-1} respectively. Accurate atomic masses are 1.007825 *amu* and 2.0140 *amu* for ^{1}H and ^{2}H respectively. The mass of ^{35}Cl is 34.96885 *amu*. Based on this information alone, can you conclude that the bond lengths are the same or different in the two molecules?