Constructing and Using Molecular Orbital Correlation Diagrams

In this exercise, you will be constructing molecular orbital diagrams of some exotic molecules that cannot be formed easily in the lab in order to predict their properties and reactivity.

The species we'll be looking at are H, He, $He_2{}^{0/2+}$, H_2, and HeH.

1. First, draw the energy levels of the 1s orbitals of hydrogen and helium on the same graph. Use their relative positions as the starting points for all of your correlation diagrams. To aid you in placing them relative to each other, $IE_H = 13.6$ eV and $IE_{He} = 24.6$ eV

2. Draw correlation diagrams for $He_2, He_2^{2+}, H_2,$ and HeH on the same energy scale. If you need the space, it may help to turn your paper sideways so they can all fit on the same line. Take time using a ruler to make the antibonding orbitals slightly farther away from the starting atomic orbitals than the bonding orbitals just as we have seen in class. For the heterodiatomic molecule, use the point halfway between the atomic orbitals as your midpoint.

3. Determine the bond order of each species.

4. Rank the species in order of stability. To do this, you will be using a ruler. We can approximate the energy of a molecule as the sum of the energies of each individual electron. If you define a common zero point (which you are doing on your diagrams), you can estimate the overall energy with a ruler. That is, electron energy can be measured in the number of cm an electron is away from zero. The farther below it is, the lower its energy, and the more stable it is. The total stabilizing energy will be the sum of all the distances that all of the molecule's electrons are away from zero.

   Hint: If you did it right, the stabilization energy of He_2 should be slightly less than 2 individual He atoms.

5. Using your answers for **1-4**, explain why the HeH molecule is unstable with respect to the following chemical reaction:

$$2 \, HeH \rightarrow \ H_2 + 2 \, He$$
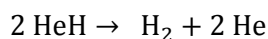
   Note: We often speak of an individual molecule as being stable or unstable, but that is a lazy shortcut for the true meaning of the word. Something can only be called stable or unstable with respect to something else (*i.e.*, something that it is more or less stable than). Therefore, in explaining question **5**, your answer must make an attempt to explain why the ΔE_{rxn} for the reaction above is less than zero.