1 Cognitive reasoning in the chemical sciences 5.5

Molecular orbital (MO) diagrams in chemistry texts are traditionally written in the *outside-to-inside* format: the starting orbitals are presented on the left and right sides of the MO diagram and the actual MOs are placed in the center.

In class, we presented to you for a first time the *left-to-right* format for MO diagrams, where initial orbitals are placed on the left, intermediate orbitals go in the middle, and the final MOs appear on the far right-side.

1. The rule for making left-to-right MOs are as listed below. Respect these rules and MO diagrams will hold no secrets from you.

   (a) Draw the initial orbitals, often, but not always the AOs, on the far left side of a landscape-oriented sheet of paper.

   (b) Remember that we can only mix orbitals one pair at a time, and that once we choose a pair, if we add some of orbital **a** to orbital **b**, then the second mixed orbital must be the subtraction of some of orbital **b** from orbital **a**.

   (c) As your diagram progresses, you will be mixing orbitals a pair at a time. Each intermediate column though should carry over orbitals not used in the last mixing process: *each intermediate column of orbitals should have the same number of orbitals as the intial left-hand-most column.*

   (d) You want to think ahead. In the lower right hand corner of your page, draw the orbital which is the lowest energy orbital that you can think of. Draw the highest energy orbital in the upper right hand corner. These are the ultimate goals of your orbital mixing. It may take several steps to get there. Whatever mixing you do, you should have as a goal the final making of these two orbitals.

   (e) You will find it easiest if your mixings respect the symmetry of the initial molecule. If two atoms are in chemically identical environments, add and subtract these orbitals in the initial intermediate stages of your diagram.

   (f) Whenever you think that you have achieved an MO, place a rectangular box around the orbital.

2. Please, using the guidelines written above, draw left-to-right MO diagrams for the following chemical systems:

   (a) The water molecule.

   (b) The hypothetical molecule BeH_2. Use VSEPR to figure out the shape of this molecule.

   (c) H_3, an unstable molecule with three hydrogen atoms in a chain.

   (d) H_4, a hypothetical molecule with four hydrogen atoms in a perfect square.

   (e) The oxygen molecule.

   (f) C_2

   (g) HCCH, acetylene. Remember to use your knowledge of Lewis structures and VSEPR to determine the correct acetylene molecular shape.