1 Cognitive reasoning in the chemical sciences 6.2

1. The rules for making *left-to-right* MOs are as listed below. In this sheet, we will tackle left-to-right MO diagrams in a different way. Rather than deriving the final MOs from the initial AOs, we will derive the final MOs from the Lewis structure. Start by drawing the Lewis strucuture. From this Lewis structure deduce the hybrized orbital energy diagram. And from these hybridized orbitals, using the left-to-right MO diagram rules, deduce the final MO diagram.

   The left-to-right MO diagram rules:

   (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 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 these rules together with the procedure written above, draw left-to-right MO diagrams for the following chemical systems:

   (a) The water molecule.

   (b) The hypothetical molecule BeH_2.

   (c) The carbon dioxide molecule.