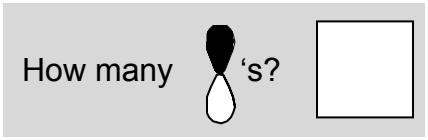
Chemistry 2302 Tuesday, June 17

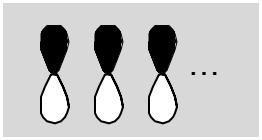
In-Class Exercise:
Molecular Orbital Diagrams of Conjugated Systems

In the last lecture, we discussed the molecular orbital diagram for a conjugated diene. In this exercise, you'll use the guidelines we discussed to draw a diagram for 1,3,5-hexatriene.

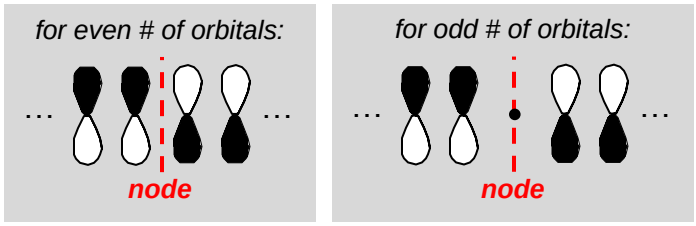
1. How many *p* orbitals in a row does this molecule have? That's how many molecular orbitals you will end up with.



2. At the bottom of the energy scale on the next page, draw a molecular orbital in which the phase of all of the orbitals is the same (where there are no antibonding interactions).



3. Now, above this orbital in energy, draw an orbital that has one node in the middle. (If you had an odd number of atoms and *p* orbitals, the node would be on top the central atom, and there would be no orbital contribution from that atom. But here you have an even number of *p* orbitals, so that doesn't happen here.)



4. Keep drawing molecular orbitals up the energy scale, with each orbital having one more node than the one below it.

5. For each of the orbitals you've drawn, count how many bonding and how many antibonding interactions there are. If the non-bonding energy level represents the point at which the number of bonding and antibonding interactions match, which of your orbitals are below this level? Which are above?

6. Now fill your molecular orbitals with electrons. How many conjugated *p* electrons are there in 1,3,5-hexatriene? Where will they go in your diagram?

Molecular Orbital Diagram: