GTQ on Structure, Orbitals and Bonding
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(1) Let's look at some standing waves on a square surface (drums). The base tone would have no node and the entire surface would always swing in phase (entire surface on one side at a time). Any idea how we could get overtones? Draw the standing waves of the first few overtones and clearly indicate the nodes. Indicate + and - regions of the amplitude. (What do the results have to do benzene?)

(2) More on nodes. Review the stuff on nodal properties in the handout and think about the types and number of the nodes in these orbitals: Atomic orbitals of the types 2s, 2p, 2s and 3p. Molecular orbitals: σ and σ* in ethane, σ and σ* in ethene, π and π* in ethene and in ethine.

(3) As we have seen in the lecture, the VB method works just fine for all those molecules *without* multiple bonds. Once there are multiple bonds, we need to invoke such concepts like resonance. This is one of the major reasons why chemists like to separate σ and π bonds. The former can always be treated well with VB theory, the latter require either LCAO theory or resonance. So we need to make da---- sure that we know what σ and π bonds are. Do you know?

(4) Which is more bonding: σ or π bond in C_2H_4? Why? (explain with "overlap")

(5) Hybridization: Very basic stuff that you need to know!! Look at as many structural formulas in the book as possible and determine for each bond what AOs are involved. This is best done in small groups (have some fun competition).

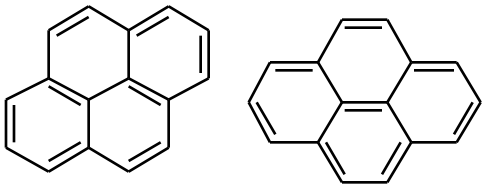
(6) The construction of the sp AOs is the simplest and this can be done without much math (in fact without any). Can you do it?

(7) What are the rules that we need to follow to generate the ground state of a molecule given an MO energy level diagram? Some of these rules also hold for excited states, others don't. Which do, which don't? Draw the energy level diagram for benzene. Draw the ground state and also draw a couple of excited states.

(8) Know your CC bond lengths! This is an order (well meant).

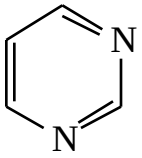
(9) Look at the list of functional groups on the inside of the back cover of V&S. Go down the list of functional groups and think about the polarization of each bond. What direction, how much (relatively speaking).

(10) Draw *all* resonance forms of these molecules. Give the ordering of their importance. Which one is more stable?

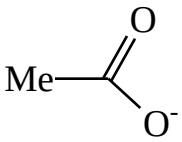


(11) Give the structure of an open-chain five carbon compound with (a) two double bonds in conjugation; (b) two isolated double bonds. (More than one answer might be possible.)

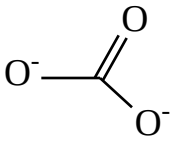
(12) Show all resonance forms for the following structures.



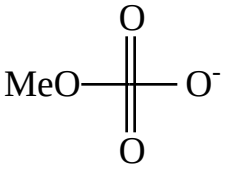
pyrimidine



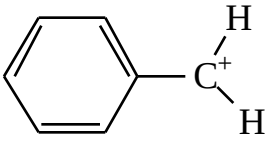
acetate



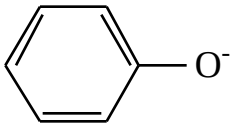
carbonate



methylsulfate



benzyl cation



phenolate anion