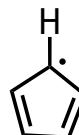


Organic Chemistry - Exercise 2

Distribution: September 26 2024

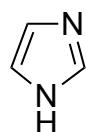
Help: October 3 2024

Return until: October 7 2024

1. Consider the compound $(CH_3)_2B-N(CH_3)_2$ that contains a B-N bond.
 - a. Use the VSEPR model to explain what hybridization states you would **expect** for B and N, respectively.
 - b. **Experimentally**, you can show that the N atom has a trigonal-planar coordination geometry (to the B and the two C atoms). What does that mean for its hybridization state?
 - c. Draw a VB model and two (Lewis) resonance structures of the molecule. What do you expect the bond order of the B-N bond to be? What do you expect for the dipole moment of this molecule?
 - d. Draw a simplified MO diagram of the molecule.
2. The cyclopentadiene radical is a **planar molecule** with the molecular structure represented below (the dot is an unpaired electron):


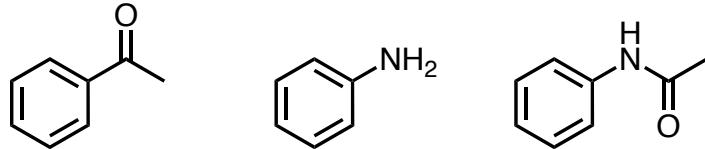
 - a. What is the hybridization state of the carbon atoms ? How many carbon atoms contribute to the π MO system? How many π MOs are formed? How many π electrons are involved ?
 - b. Establish a simplified MO energy diagram of the π MO system (ignore all C-C and C-H σ bonds) according to the Hückel model for monocyclic compounds
 - c. Use the 'electron in periodic box' model ('steady boundary condition') to find out how the different carbon p AOs contribute to the different MOs !
 - d. From your previous answer, draw simplified LCAO representations of the different MOs in the cyclic molecule.
 - e. Discuss whether the molecule is aromatic or not and comment on its preferred reactivity. Discuss whether or not the cyclopentadienide anion is aromatic or not.

3. Imidazole is a heterocycle comprising two non-adjacent (and different!) nitrogen atoms. Its structure is shown below.



- a. Experimentally, it is shown that the molecule is fully planar. What does that mean for the hybridization of the two nitrogen atoms?
- b. In what type of atomic or hybrid orbital is the free electron pair located in each of the two different nitrogen atoms? Briefly explain why.
- c. Draw two additional resonance structures of imidazole.
- d. How many π orbitals does imidazole form? How many π electrons does imidazole possess?
- e. The Hückel rule for aromaticity refers to planar, cyclic systems comprising $4n+2$ π electrons. With this in mind, discuss whether imidazole is aromatic or not.

4. The structure of benzaldehyde, aniline and acetanilide are shown below:



- a. Draw all relevant resonance structure for the three compounds.
- b. Comment on the mesomeric effect of the different substituents attached to benzene of the three compounds and then compare the different electron density of the benzene rings.

Reading Suggestions:

Clayden, Greeves, Warren, Wothers, *Oxford University Press*, **2001**, pp. 20-45 ; 81-110 & 151-179.

Organic Chemistry, John McMurry, *Thomson Brooks/Cole*, **2008**, pp. 1-48 & 73-110.

Chimie Organique, Paul Arnaud, *Dunod Editeur*, **2015**, pp. 73-103 & 161-188.