

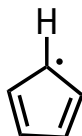
Organic Chemistry - Exercise 2

Distribution: September 26 2024

Help: October 3 2024

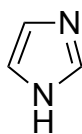
Return until: October 7 2024

1. Consider the compound $(\text{CH}_3)_2\text{B}-\text{N}(\text{CH}_3)_2$ 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):

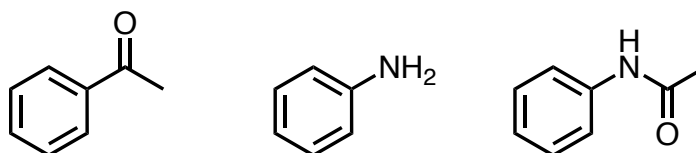


- a. What is the hybridization state of the carbon atoms? How many carbon atoms contribute to the π MO system? How many π MOs are formed? How many π electrons are involved?
- b. Establish a simplified MO energy diagram of the π MO system (ignore all C–C and C–H σ bonds) according to the Hückel model 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.



- Experimentally, it is shown that the molecule is fully planar. What does that mean for the hybridization of the two nitrogen atoms?
 - 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.
 - Draw two additional resonance structures of imidazole.
 - How many π orbitals does imidazole form? How many π electrons does imidazole possess?
 - 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:



- Draw all relevant resonance structure for the three compounds.
- 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.