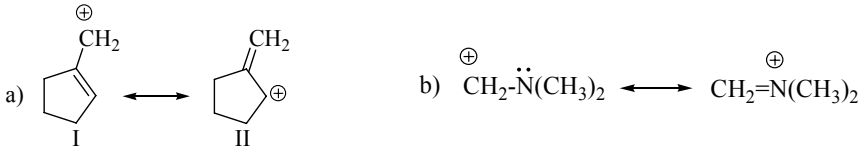
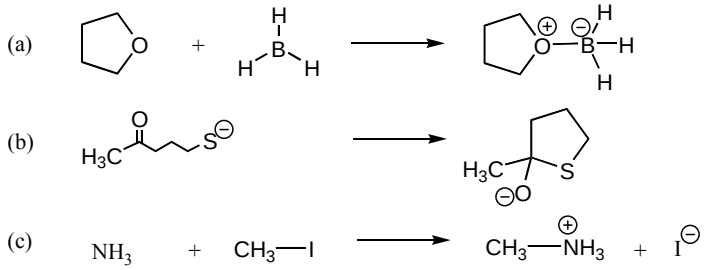
CH105: Organic Chemistry: Tutoral-2

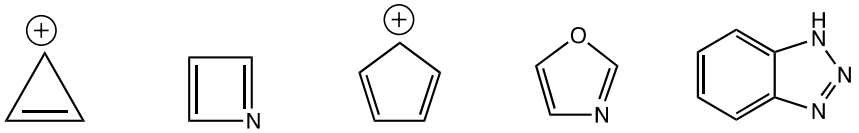
1. From each of the resonance structures that follow, designate the one that would contribute most to the hybrid and explain your choice.



2. In each of the given cases, identify (i) the nucleophile and the electrophile (ii) show using 'electron-pushing' arrows how the following reaction happens (iii) what kind orbitals (such as n, σ, σ*, π, π* or AO) of the nucleophile and the electrophile are involved in these reactions.

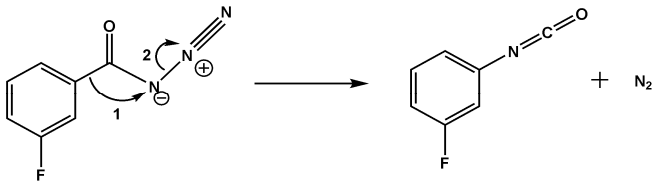


3. Label following compounds as aromatic or antiaromatic

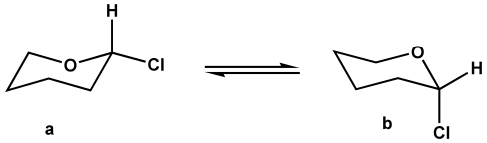


1 **2** **3** **4** **5**

4. Mechanism of a molecular rearrangement reaction (reaction in which bonds migrate) is shown below. Identify the **frontier orbitals** involved in the **first step (arrow 1)** of this rearrangement. Also identify the **type of frontier orbital interactions (σ/π)** involved in **first step** by **sketching** the orbital interaction.



5. An equilibrium is presented below.

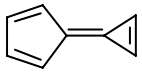


(A) Identify the **more stable equilibrium isomer**

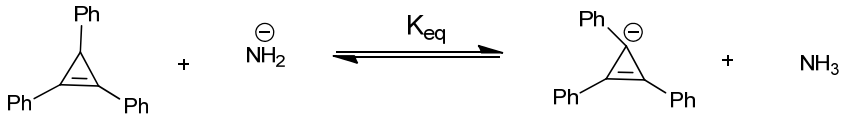
(B) Identify the **origin of orbital stabilization** of the favored conformer. (show graphical representation of orbitals to justify your answer)

6. Give reasons for the following observations,

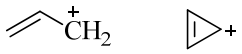
(A) The observed dipole moment of the given molecule, μ=5.6 D



(B) The equilibrium constant (K_{eq}) of the following reaction is very small,



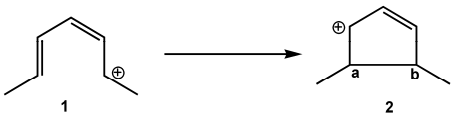
7. Deduce the MOs of cyclopropenyl cation from that of allyl cation. Comment on the degeneracy of MOs,



8. (A) Draw the occupied π-MOs of 1,3,5-hexatriene and identify the number of nodes in each MOs. (B) Explain why the lowest occupied π-MO of benzene is lower in energy than the lowest energy π-MOs of 1,3,5-hexatriene.

*9. Cation **1** undergoes ring closure reaction to form **2**.

(**A**) Based on molecular orbital symmetry considerations through the **analysis of HOMO** (show picture) provide the relative stereochemistry (cis/trans) of methyl groups at carbon a and b in **2**



(**B**) The orbital coefficients of the two of the π MOs of cation **1** are given below. Show the orbital pictures and specify which is of lower energy.

$\Psi_N = 0.5\varphi_1 + 0.5\ \varphi_2 - 0.5\ \varphi_4 - 0.5\ \varphi_5$

$\Psi_{N'} = 0.58\varphi_1 - 0.58\ \varphi_3 + 0.58\ \varphi_5$

10. (a) Draw the HOMO and LUMO of ethylene and 1,3-butadiene. (b) Identify the important orbitals that are involved in the reaction as shown below,