## **Tutorial 1**

1. Classify the following compounds as aromatic/antiaromatic/non-aromatic based on Huckel's rule.





c.







2. Identify the orbital interactions involved in the following reaction.

3. Is 'twistane' shown below chiral? Identify and pictorially show all the symmetry elements (if present).



## **TWISTANE**

4. The reaction given below passes through a five-membered transition state (TS).

- a. Draw the HOMO-LUMO of diene involved.
- b. Show **both possible** combinations of orbital interactions between diene and carbene (HOMO and LUMO given below) responsible for the product formation.







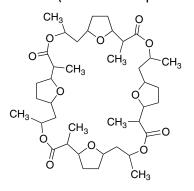
LUMO

(Note: It is an example of cheletropic reaction, which you need not know or remember for solving this question!).

5. The molecule given below is a substituted cubane. Identify: a. Total number of stereoisomers that exist; b. Total number of pair of enantiomers.



6. Shown below is the structure of nonactin without any specification of stereochemistry. It was found to be optically inactive. When completely hydrolyzed, it yields racemic nonactic acid. Draw the **stereochemical structure** of nonactin from this information using appropriate wedges at the chiral centres. (\*Take home problem)



nonactic acid

## **Tutorial 1 (Solution)**

1. Classify the following compounds as aromatic/antiaromatic/non-aromatic based on Huckel's rule.

a.







- a. non-aromatic
- b. aromatic (An sp-hybridized molecular carbon allotrope reported in 'Science' on 15 Aug 2019!)
- c. antiaromatic
- d. aromatic
- 2. Identify the orbital interactions involved in the following reaction.

$$\mathsf{H}\text{-}\mathsf{C}\text{=}\mathsf{C}\ominus \ + \ \begin{matrix} \mathsf{C}\mathsf{H}_3 \\ \mathsf{O} \\ \mathsf{O} \\ \mathsf{C}\mathsf{H}_3 \end{matrix} \underbrace{\mathsf{C}}^{\mathsf{C}\mathsf{H}_3} \\ \longrightarrow \ \mathsf{H}\text{-}\mathsf{C}\text{=}\mathsf{C}\text{-}\mathsf{C}\mathsf{H}_3 \ + \ \mathsf{H}_3\mathsf{C}^{\mathsf{C}\mathsf{O}} \\ \mathsf{C}\mathsf{H}_3 \end{matrix}$$

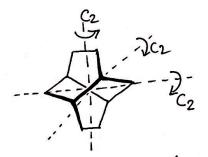
$$(n_c)^2 \rightarrow (\sigma^*_{c-o})^0$$

3. Is 'twistane' shown below chiral? Identify and pictorially show all the symmetry elements (if present).



**TWISTANE** 

(8)



(a) chiral (½ mark)

(b) 3 C2 anes as shown above (1½ marks)

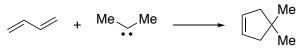
Partial wedit: just writing 3 C2 but not shown

in the diagram (½ mark)

in the diagram (1 mark)

in the diagram (1 mark)

4. The reaction given below passes through a five-membered transition state (TS).



- Draw the HOMO-LUMO of diene involved. a.
- Show both possible combinations of orbital interactions between diene and carbene b. (HOMO and LUMO given below) responsible for the product formation.

(2 marks)



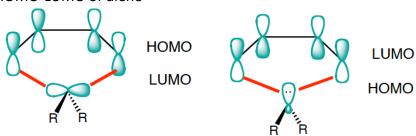


LUMO

**HOMO** 

(Note: It is an example of cheletropic reaction, which you need not know or remember for solving this question!).

## a. HOMO-LUMO of diene



5. The molecule given below is a substituted cubane. Identify: a. Total number of stereoisomers that exist; b. Total number of pair of enantiomers.



- a. Two
- b. One
- 6. Shown below is the structure of nonactin without any specification of stereochemistry. It was found to be optically inactive. When completely hydrolyzed, it yields racemic nonactic acid. Draw the **stereochemical structure** of nonactin from this information using appropriate wedges at the chiral centres. (\*Take home problem)

NONACTIC ACID - COOH . HO COOH It's enantioner's structure On hydrolysis since nonactin yields a racemic mixture, the structure has 2 molecules of NA and 2 molecules of NA\*. As nonactin is optically inactive the structure concept of will be. CH3 os Achiral as it H H3C"

CH3)

0.2