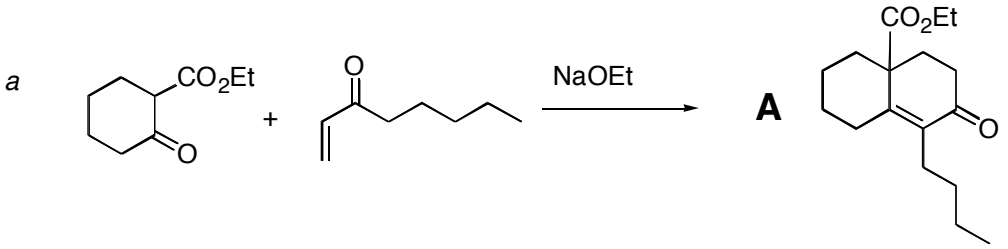
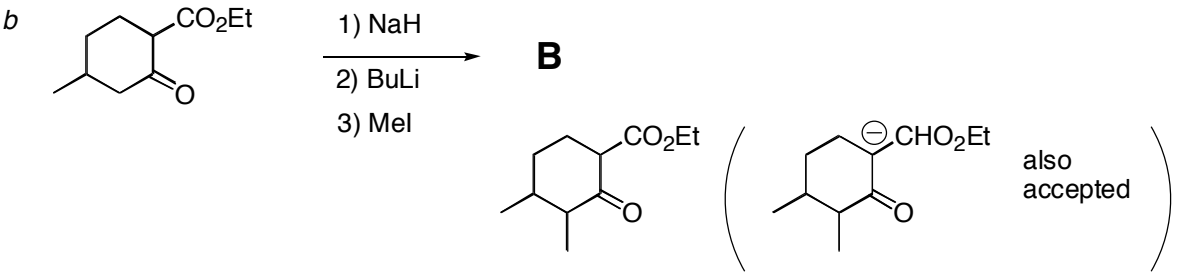
1. Provide structures of the products. Mechanisms are not needed. (5 points each)

a

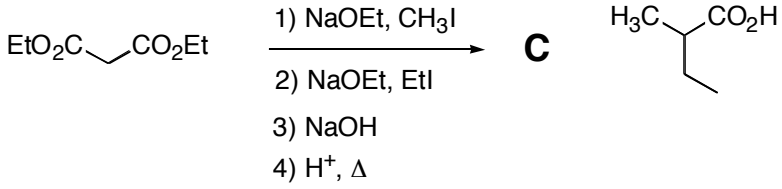


b

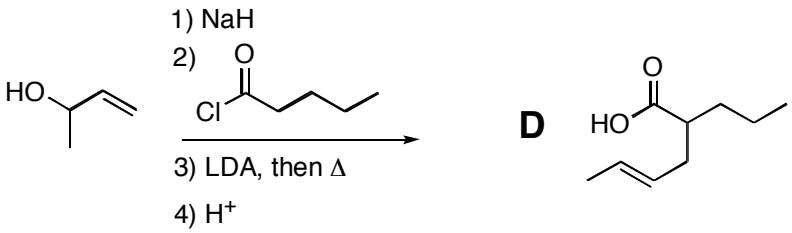


1 (continued) Provide structures of the products. Mechanisms are not needed.

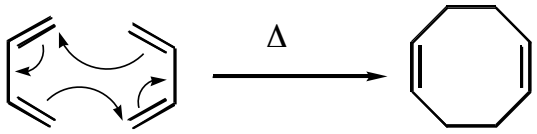
c



d

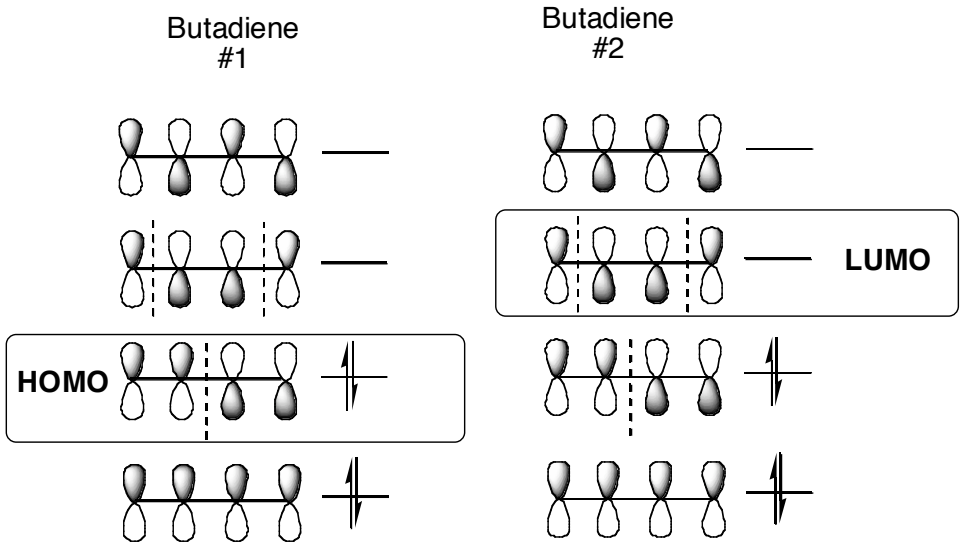


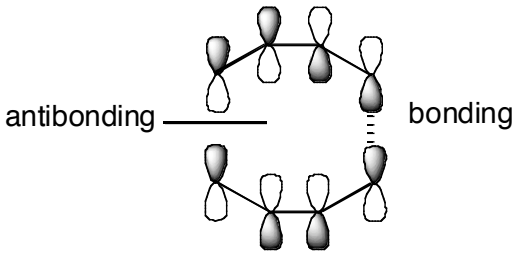
2. Consider the thermal dimerization of butadiene: (25 pts)



Would you expect this to be a concerted process under thermal conditions? Explain in detail using an argument based in molecular orbital theory.

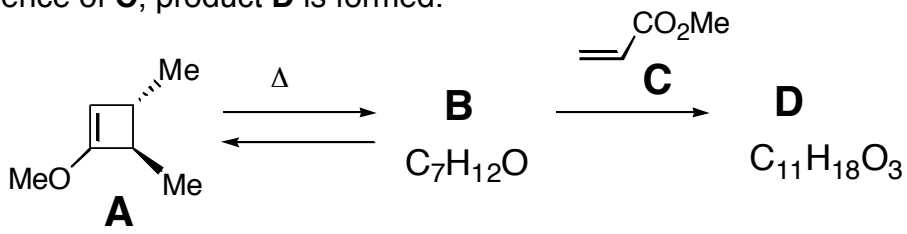
For this to be a concerted process under thermal conditions, the orbital symmetry of the HOMO of one reactant must match the LUMO of the other reactant. For the case here, we identify the HOMO of one butadiene and the LUMO of the other.



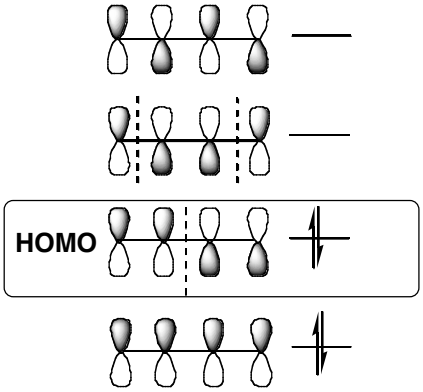


For the reaction to be concerted, we need to have bonding interactions at both termini of the reacting system. In this case, we have one bonding interaction, and one antibonding interaction. The thermal reaction does **not** take place by a concerted mechanism.

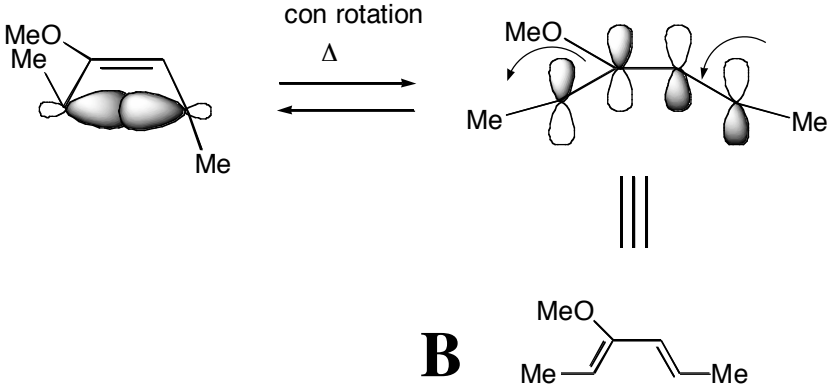
3. When heated, compound **A** reversibly isomerizes to **B**. When this process is carried out In the presence of **C**, product **D** is formed.



a. Provide the structure of **B** and an arrow pushiing mechanism for its formation. In addition, use molecular orbital theory to explain the double bond stereochemistry. (15 pts)

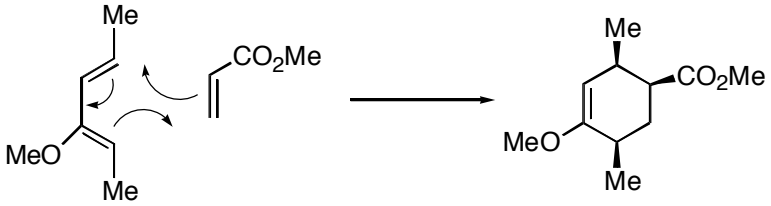


For electrocyclic ring opening/closure reactions, the reaction involves the HOMO of the diene B. **As shown on the left, the HOMO has 'unlike' symmetry, and therefore requires a conrotation in the opening. the analysis below shows that the ring opening will produce diene** B below.



B

b. Provide a structure for **D**, and an arrow pushing mechanism for its formation. Regiochemistry and stereochemistry are important! Do NOT use molecular orbitals to explain your answer (15 pts)



the 'para-like' product is formed with endo selectivity

D

4. Provide a detailed arrow pushing mechanism (25 pts)