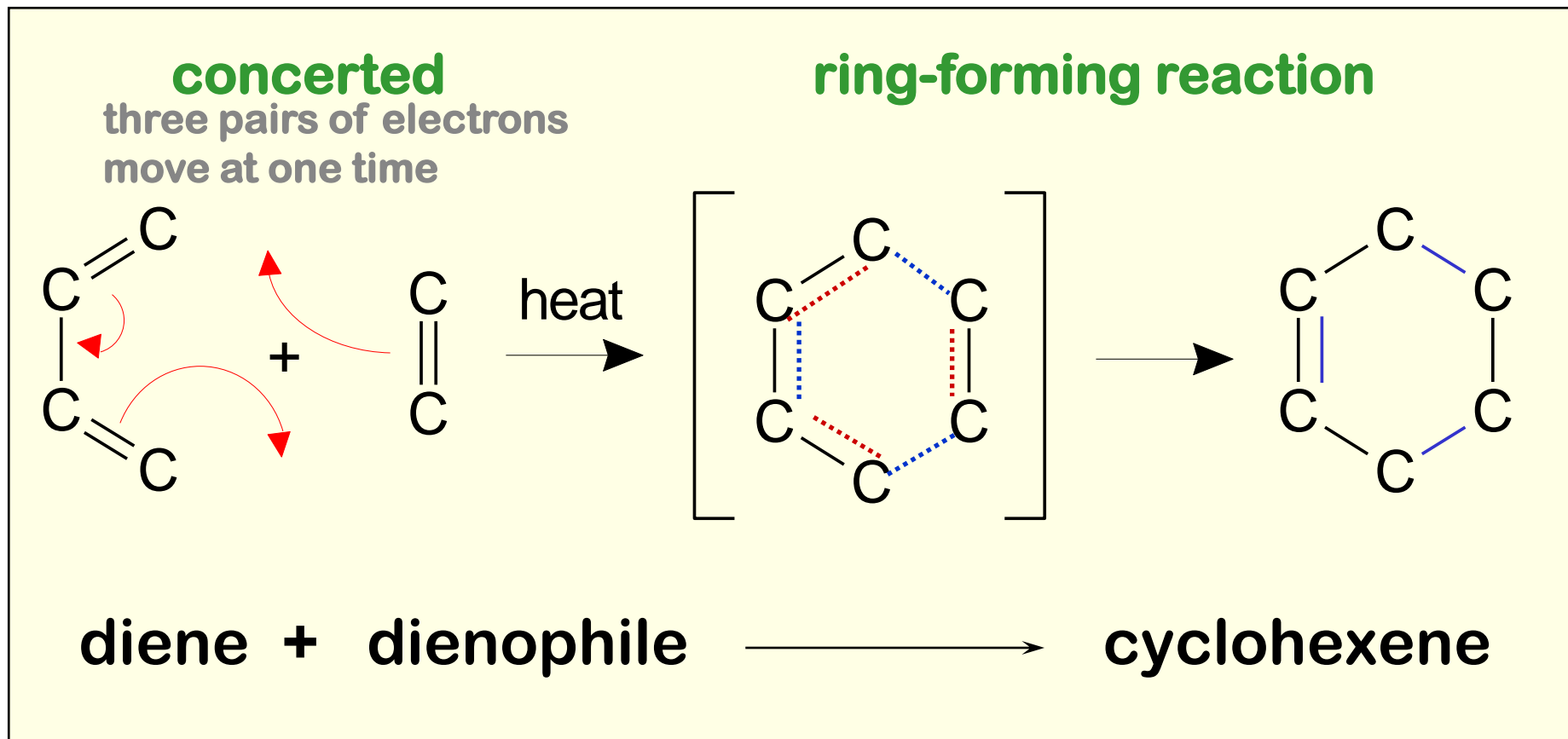


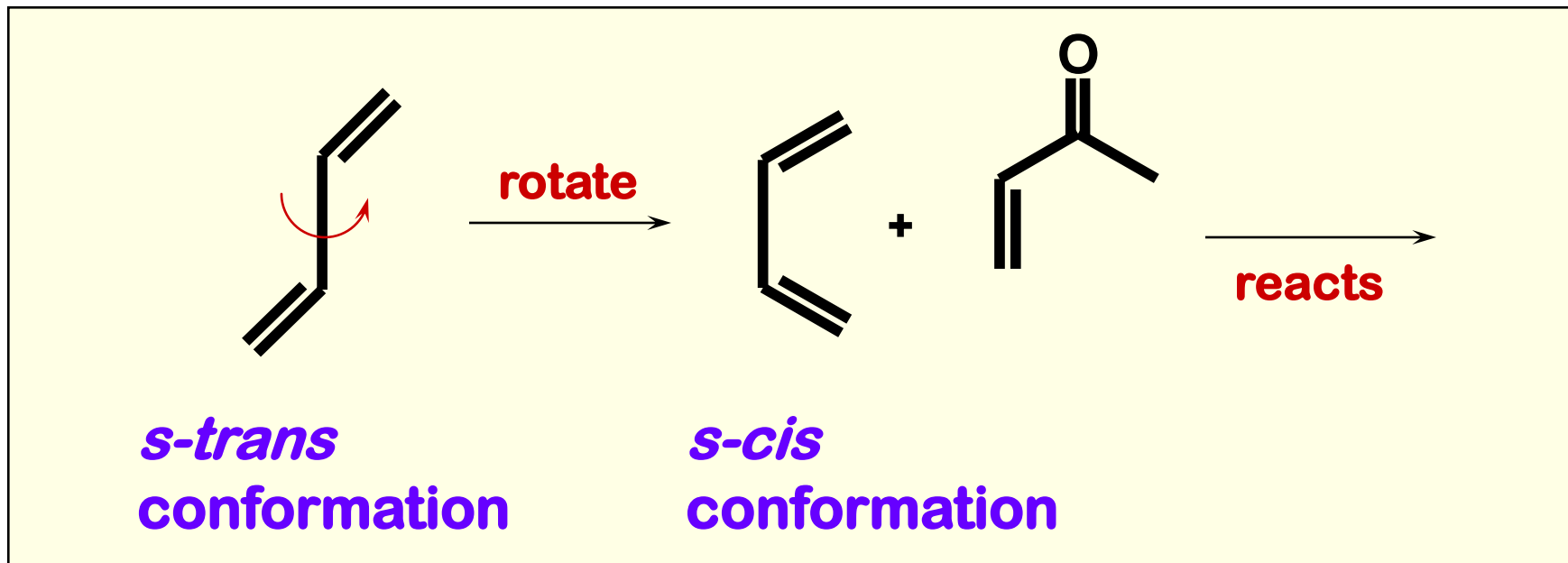
# **DIELS-ALDER REACTION**

# The Diels-Alder Reaction

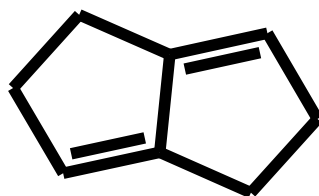


**NOTE:**  = gain of bond order  
 = loss of bond order

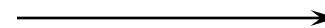
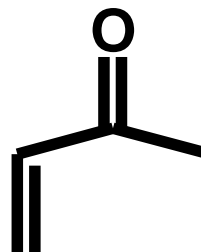
# THE DIENE MUST BE ABLE TO ADOPT THE *S-CIS* CONFORMATION



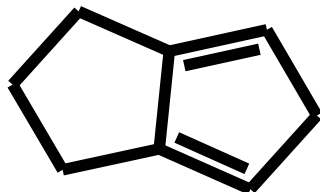
does not react



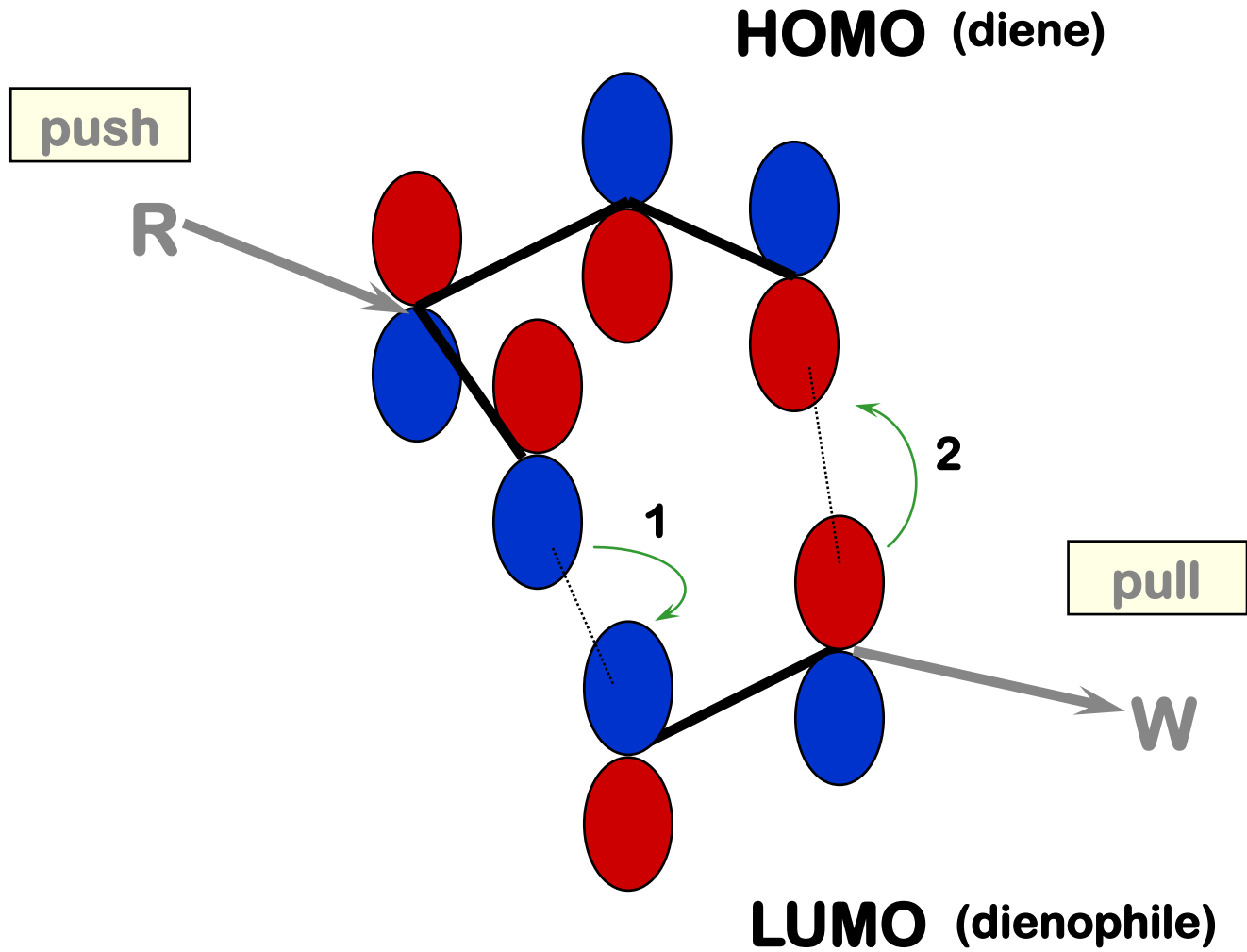
+



reacts normally



# DIELS-ALDER REACTION

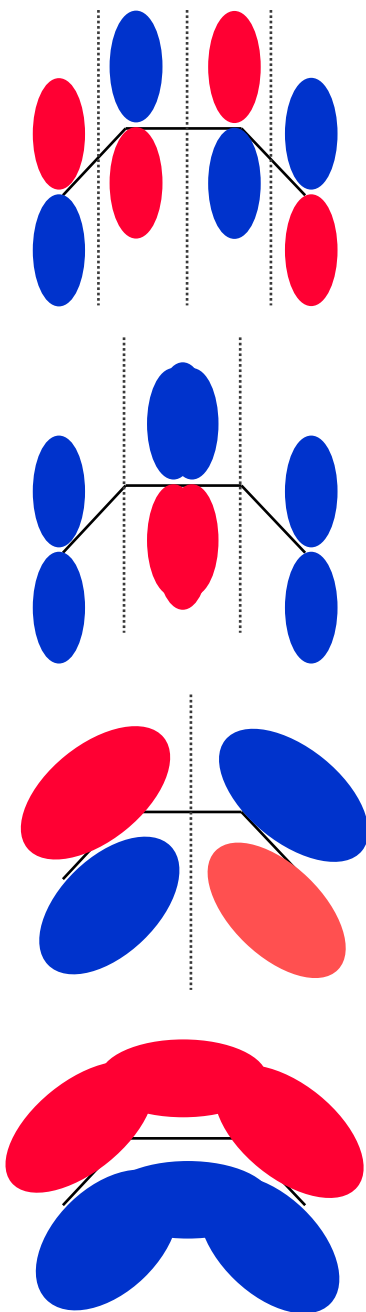


The reaction is concerted - all of the orbitals are aligned in a 6-ring.

The HOMO of the diene donates electrons into the LUMO of the dienophile.

# BUTADIENE

# ETHYLENE



$\pi_4$  \_\_\_\_\_

$\pi_3$  \_\_\_\_\_

**HOMO**

$\pi_2$   $\uparrow\downarrow$

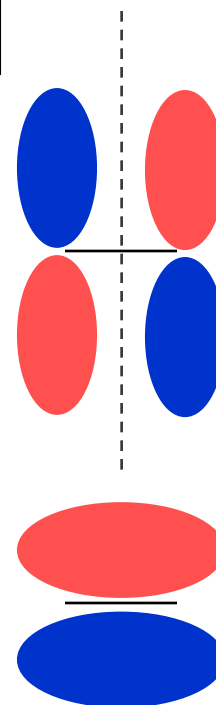
$\pi_1$   $\uparrow\downarrow$

The HOMO of the diene donates electrons into the LUMO of the dienophile.

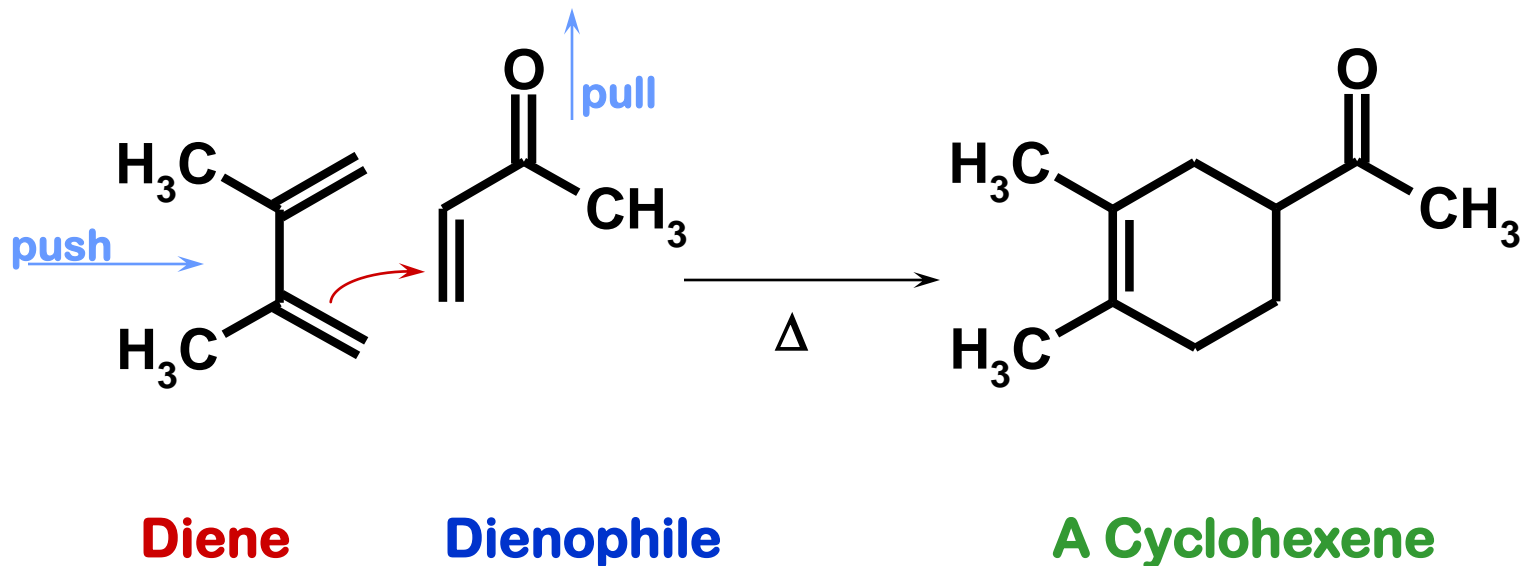
**LUMO**

$\pi^*$  \_\_\_\_\_

$\pi$   $\uparrow\downarrow$



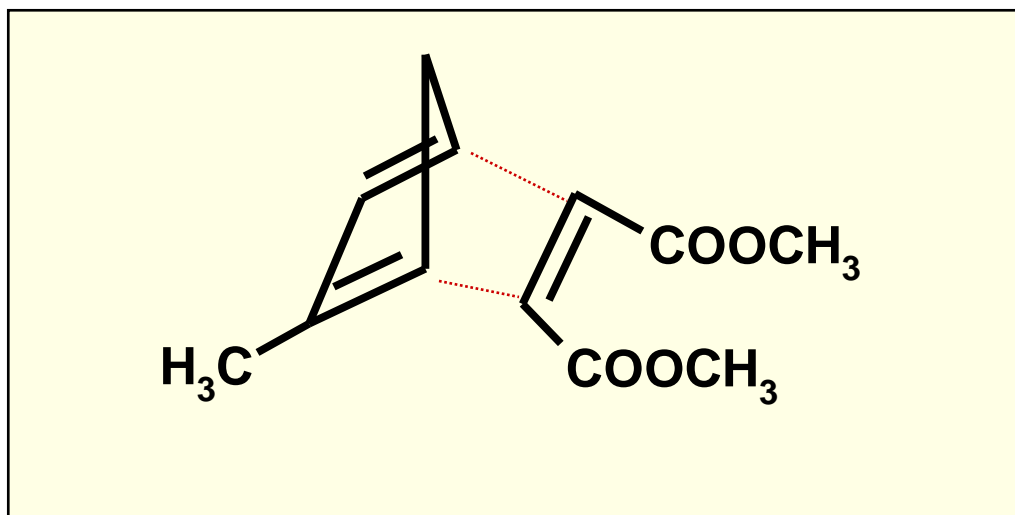
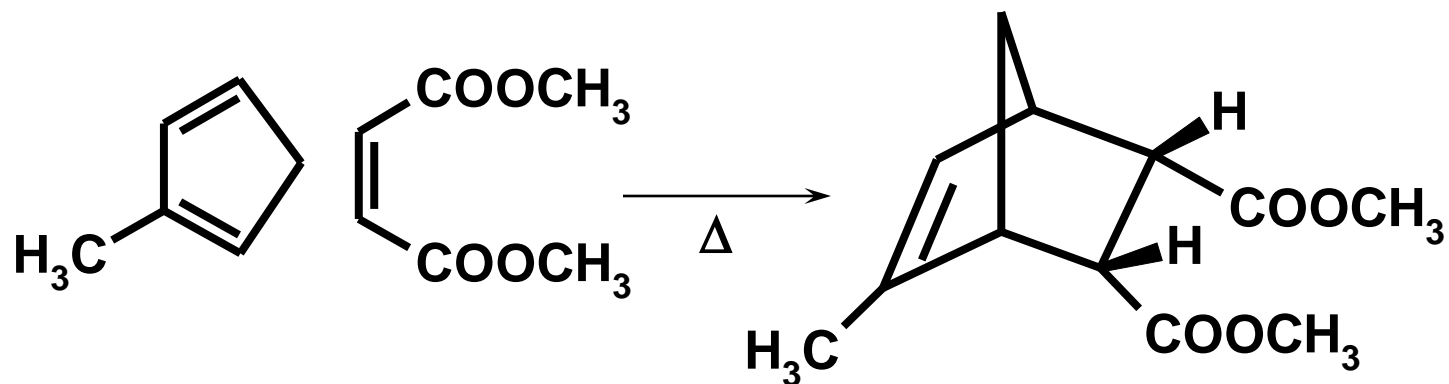
# EXAMPLE - WITH ELECTRONIC FACTORS



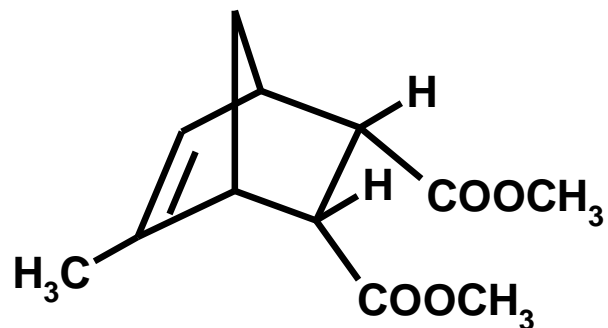
Works best if the dienophile has electron-withdrawing groups, and the diene has electron-donating groups.

The HOMO of the diene donates **PUSHES** electrons into the LUMO of the dienophile **PULLS**.

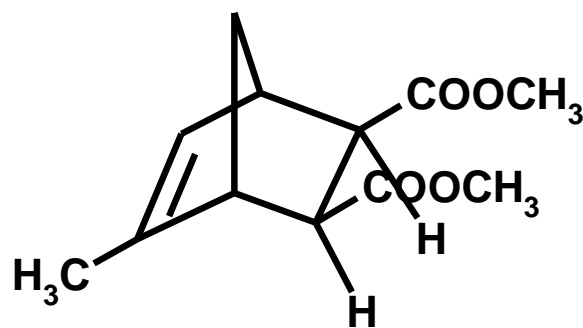
# FORMATION OF A BICYCLIC COMPOUND



# THE REACTION IS USUALLY STEREOSELECTIVE



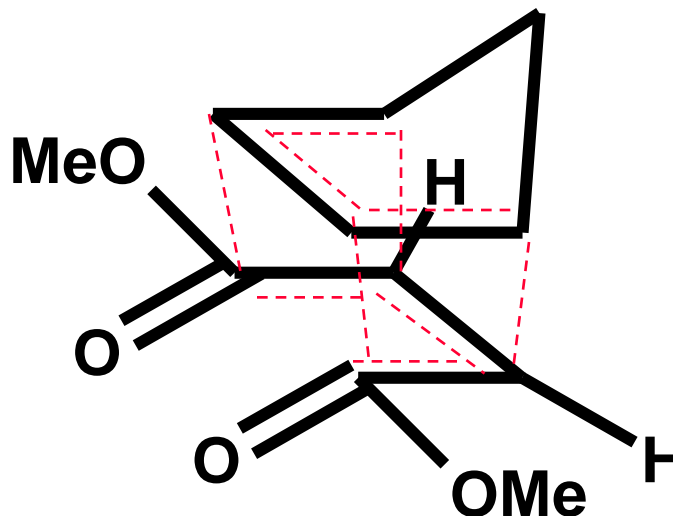
**endo**



**exo**

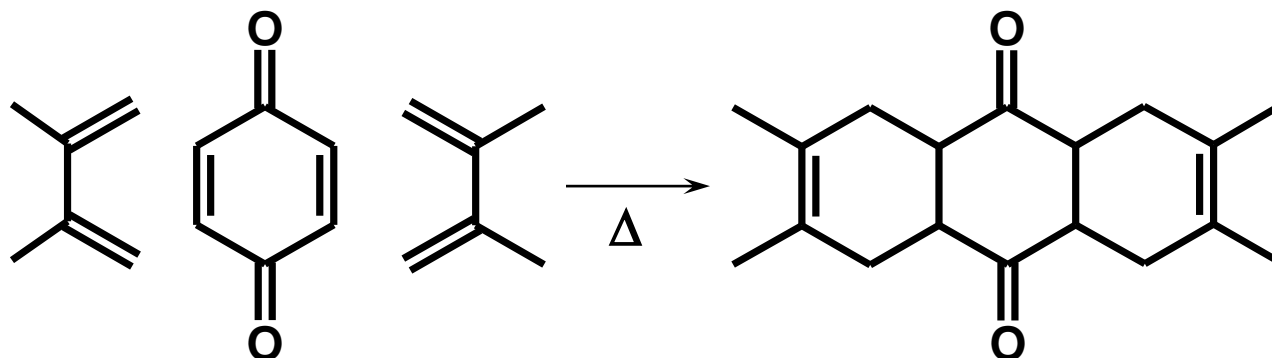
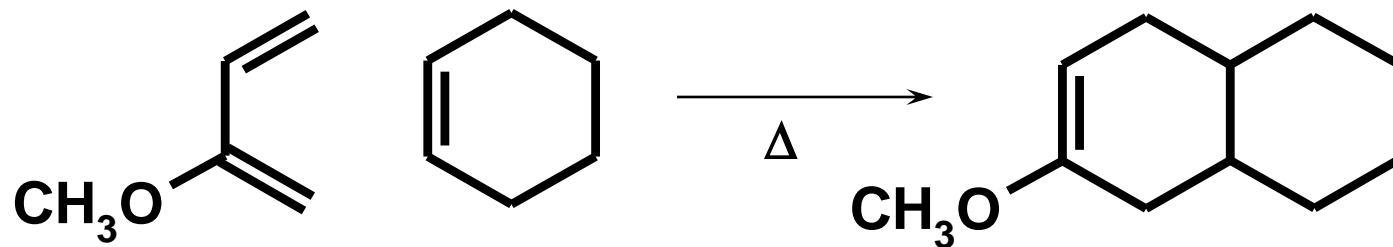
The endo product is usually preferred.

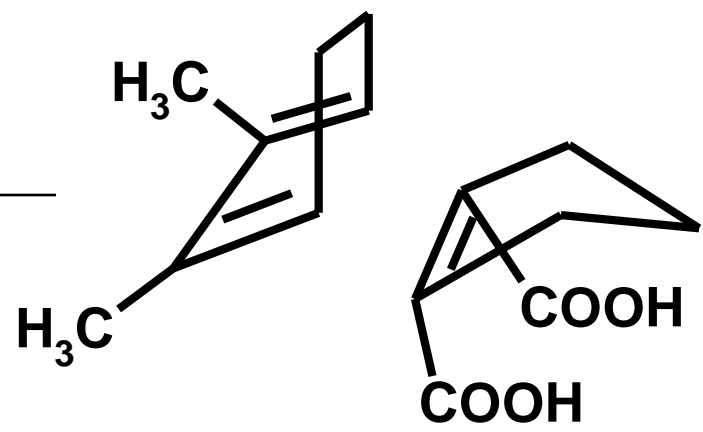
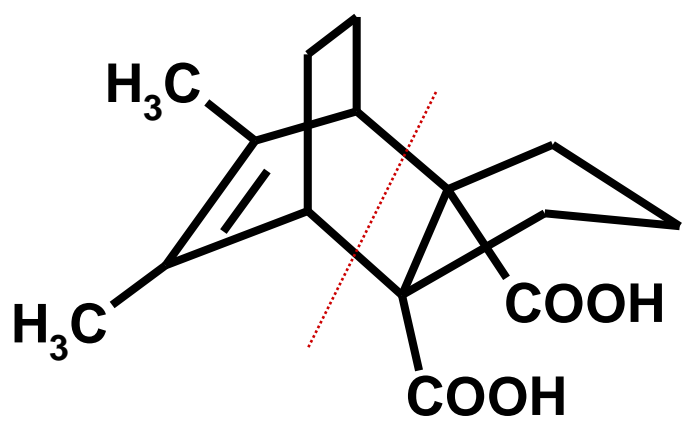
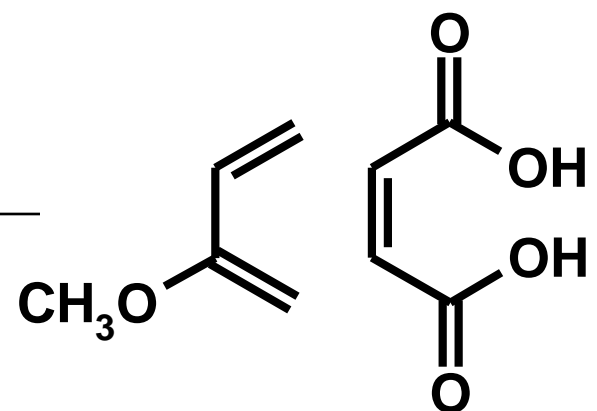
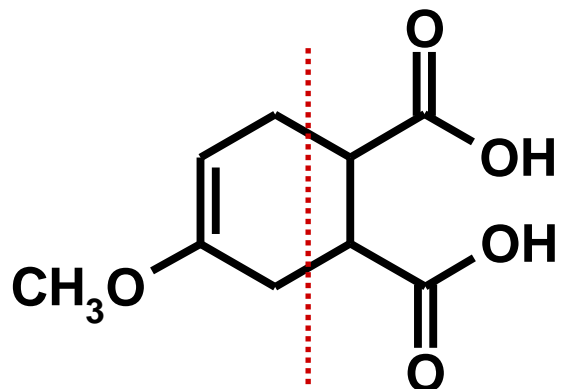
It has been suggested that the pi systems like to establish maximum overlap during the reaction.



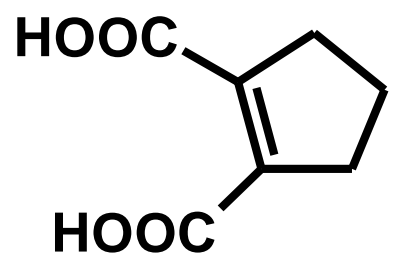
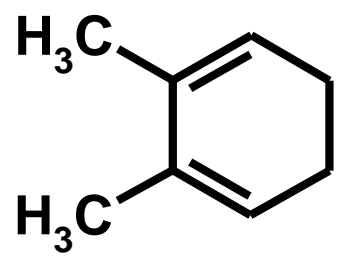


# MORE DIELS-ALDER REACTIONS



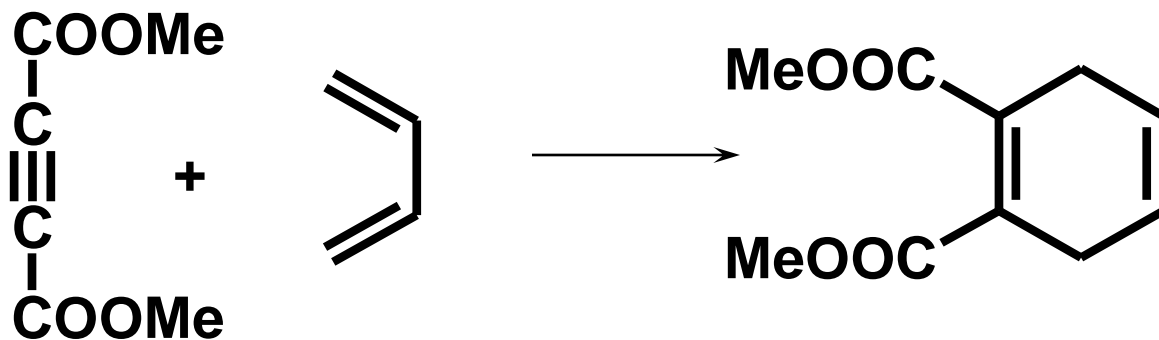


OR



**Retrosynthesis**

# ACETYLENES (ALKYNES)



**If the dienophile is an alkyne a cyclohexadiene is formed.**