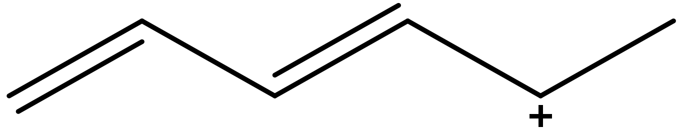
Pericyclic Reaction

Pericyclic Reactions: π-Molecular Orbital



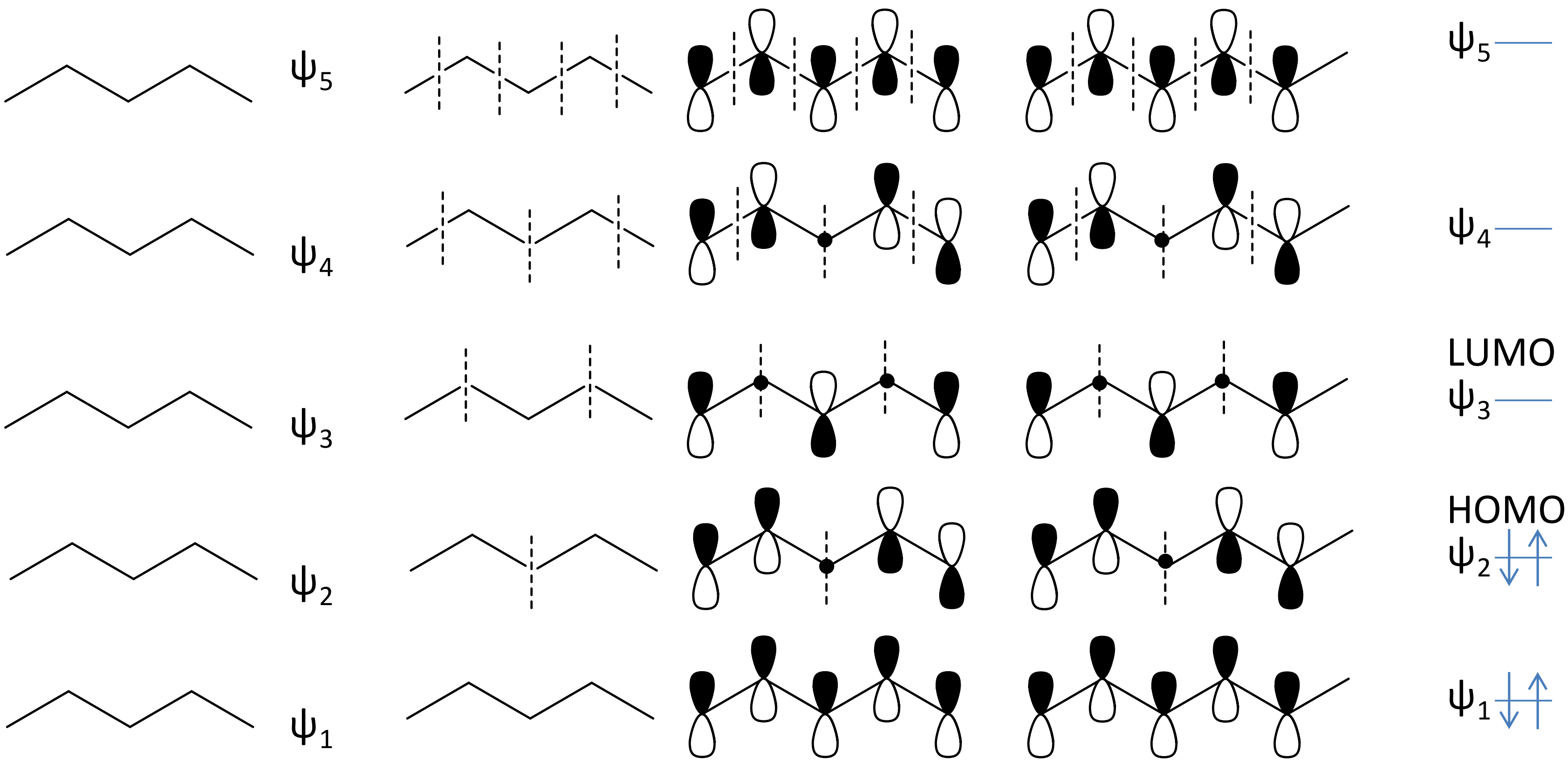
n_p is odd, $n_{BMO} = (n_p-1)/2 = 2$

$n_{AMO} = (n_p-1)/2 = 2$

$n_{NMO} = 1$

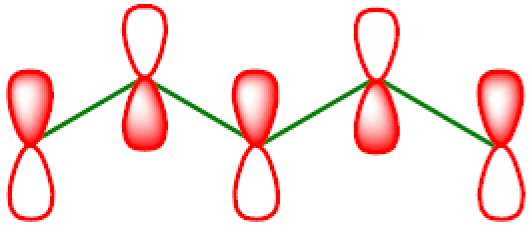
No of conjugated p orbitals (n_p) = 5

No of **π**-molecular orbitals = 5

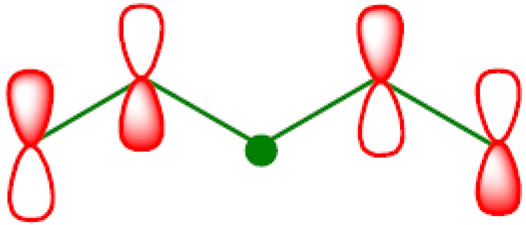


Pericyclic Reactions: π-Molecular Orbital

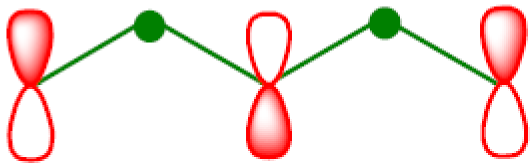
Indicate the following as BMO, AMO or NBO



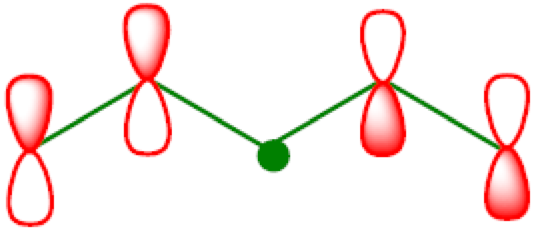
I



II



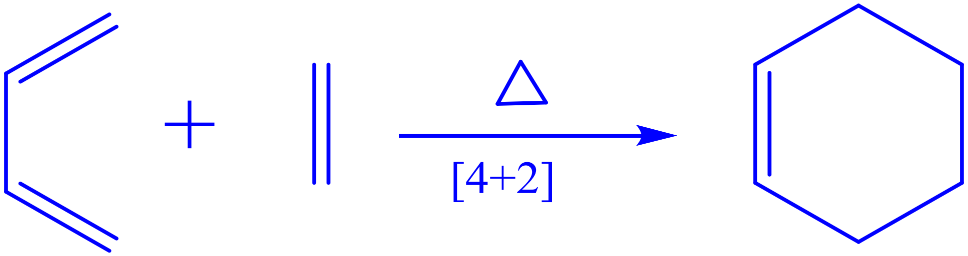
III

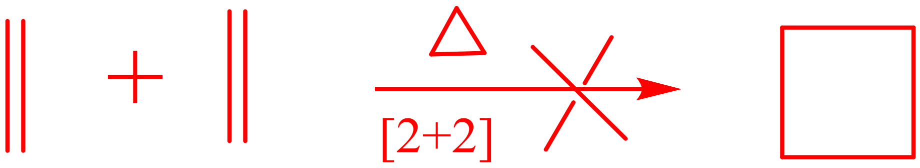


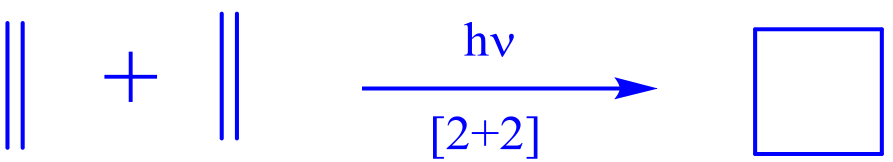
IV

Order of energy: **I>II>III>IV**

Pericyclic Reactions: Reactivity

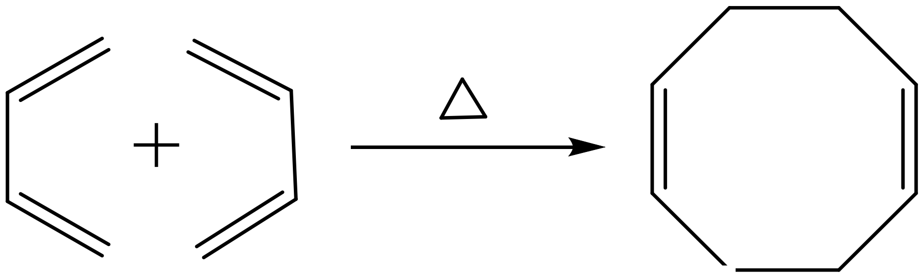


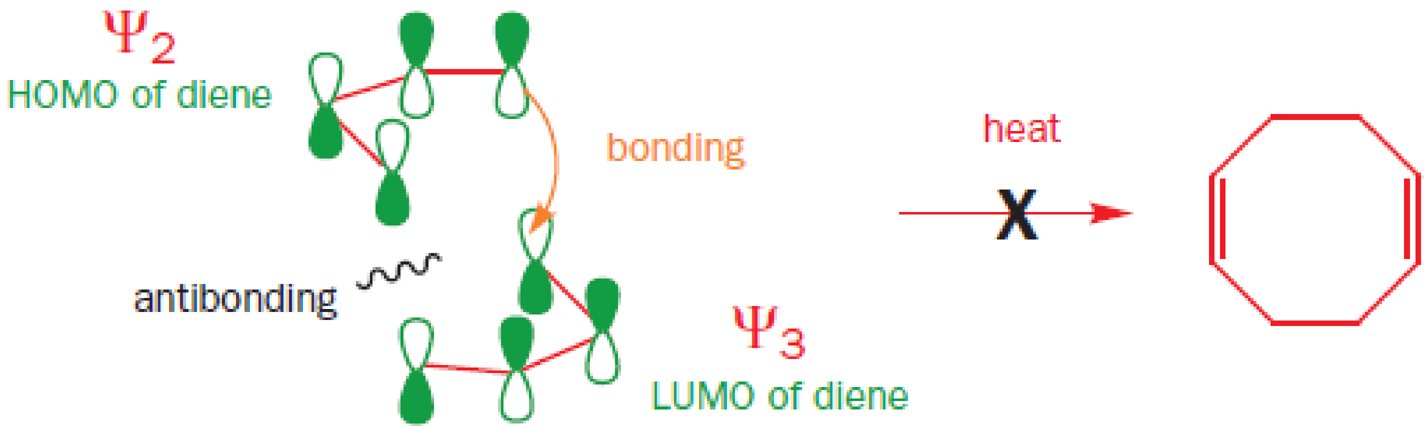


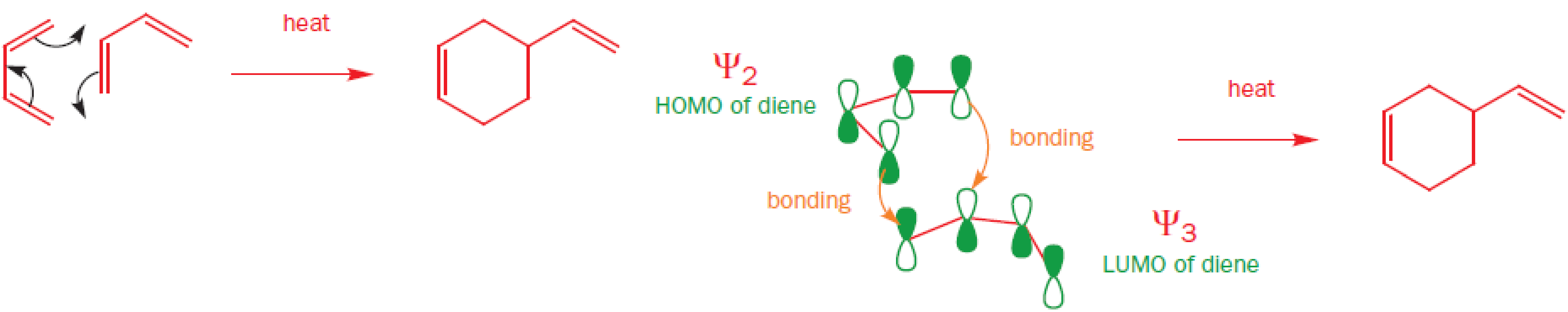


Pericyclic Reactions: Reactivity

Based on FMO theory, predict whether the following reaction is feasible or not

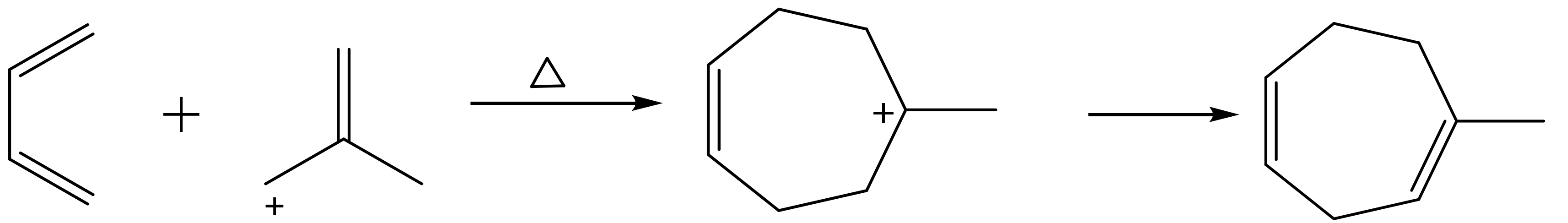




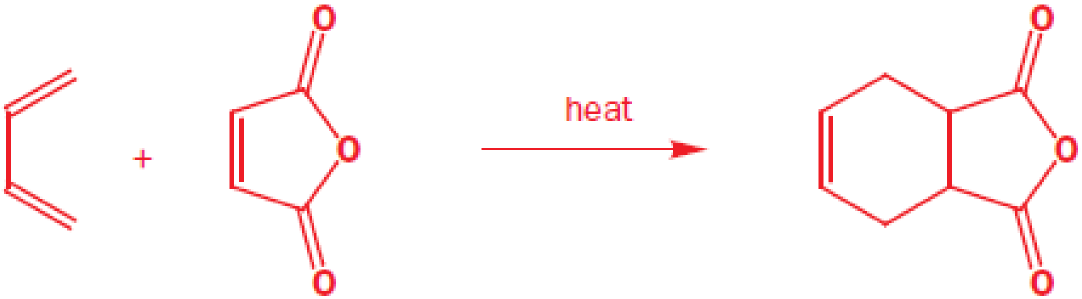


Pericyclic Reactions: Reactivity

Based on FMO theory, predict whether the following reaction is feasible or not



Pericyclic Reactions: Selectivity of Diels-Alder Reaction



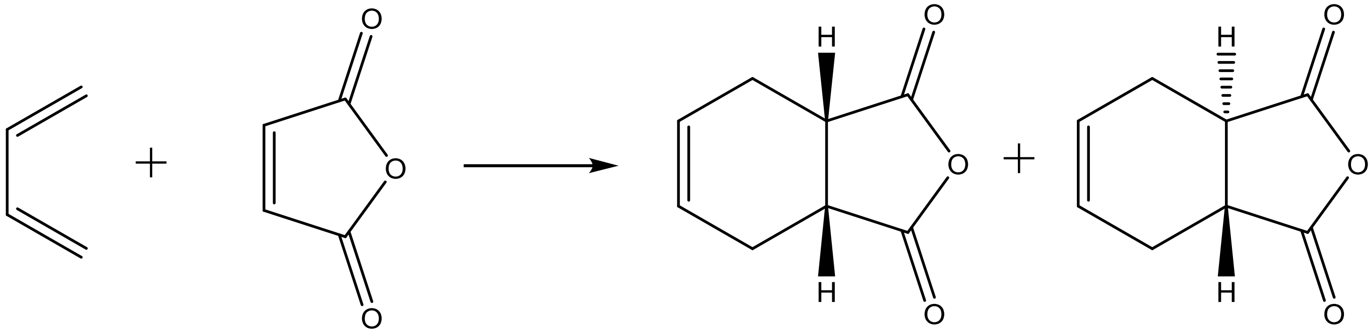
Diene Dienophile

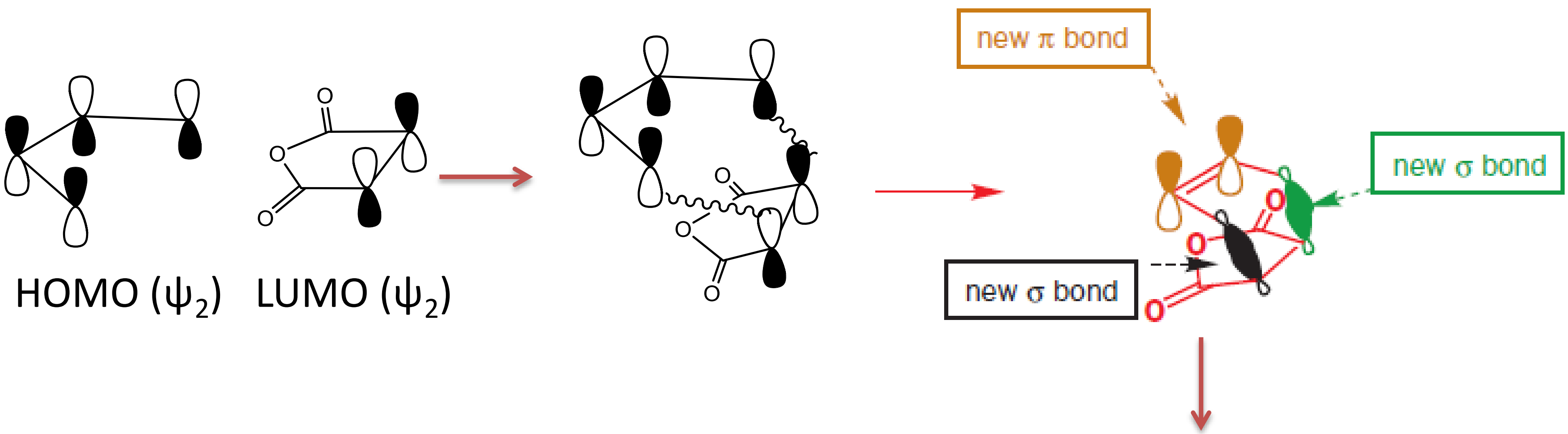
worked at the University of Kiel and discovered this reaction in 1928. They won the **Nobel Prize** in 1950.

Otto Diels (1876–1954)

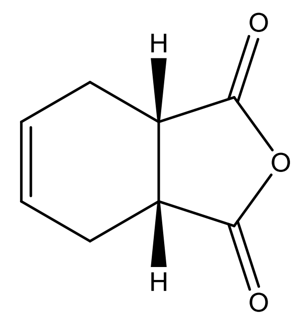
Kurt Alder (1902–58)

Pericyclic Reactions: Selectivity in Diels-Alder Reaction



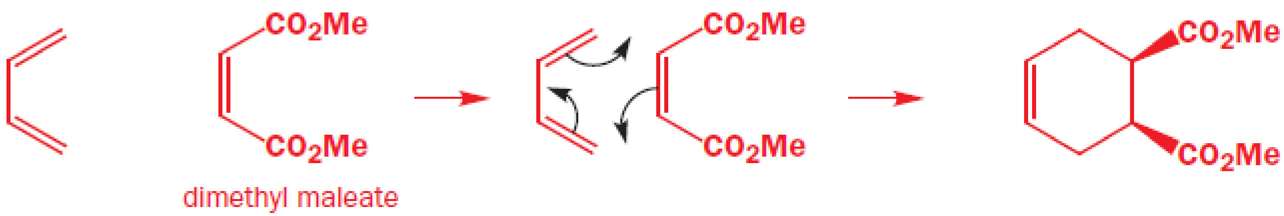


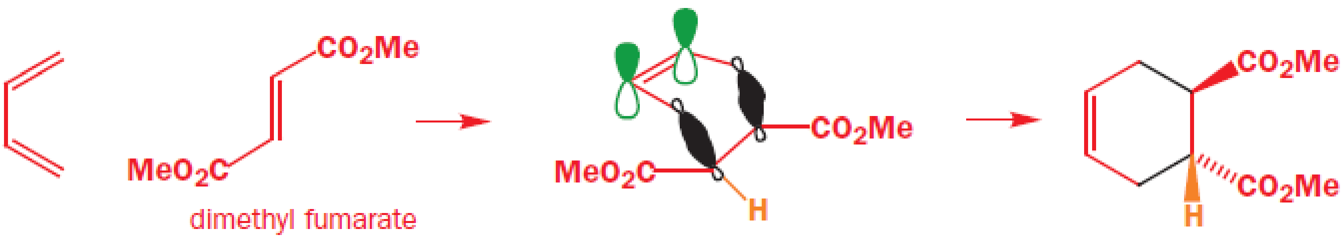
Geometry of dienophile retained



Only *Cis*-product

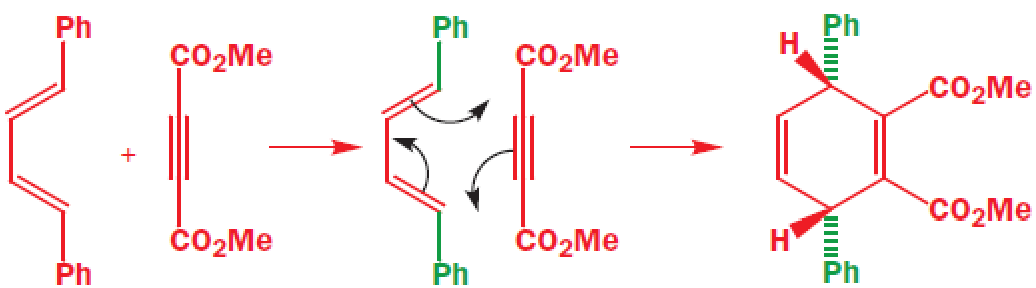
Pericyclic Reactions: Selectivity in Diels-Alder Reaction

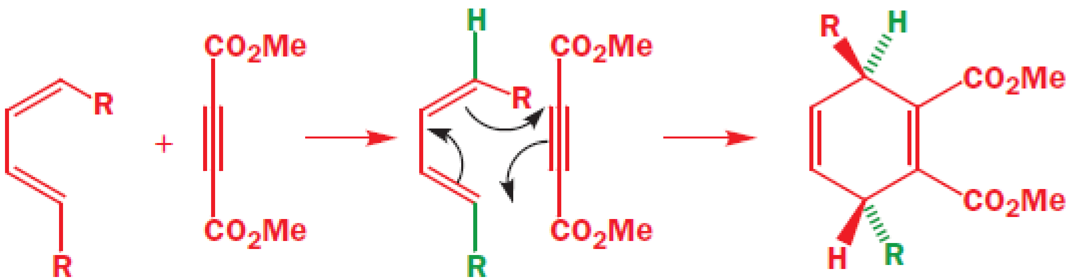




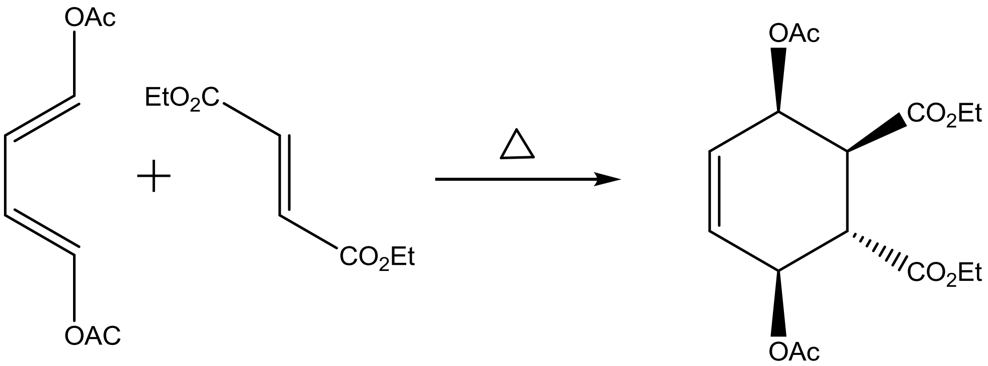
Geometry of dienophile is retained: cis-alkene give cis-product

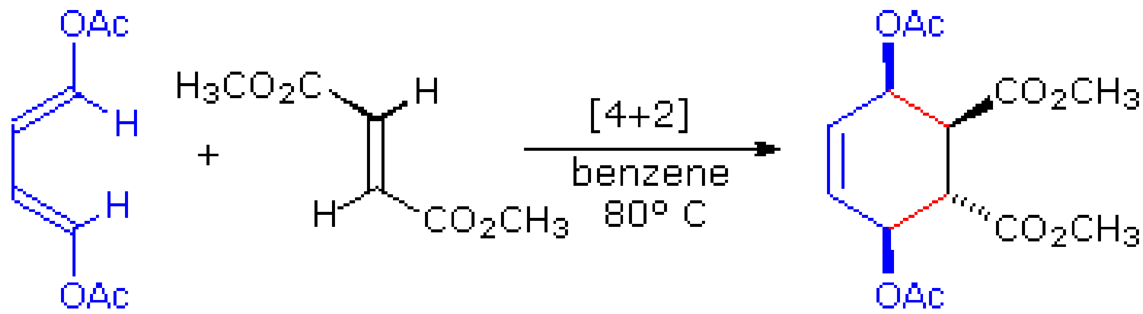
and trans-alkene gives trans-product

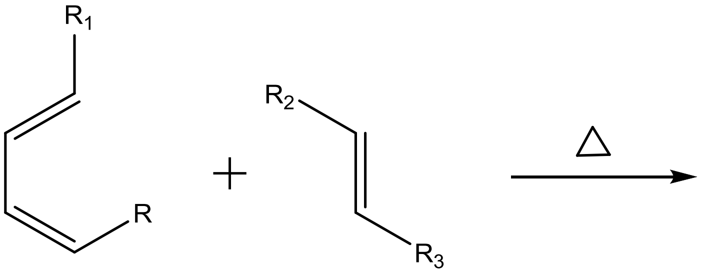




Pericyclic Reactions: Selectivity in Diels-Alder Reaction

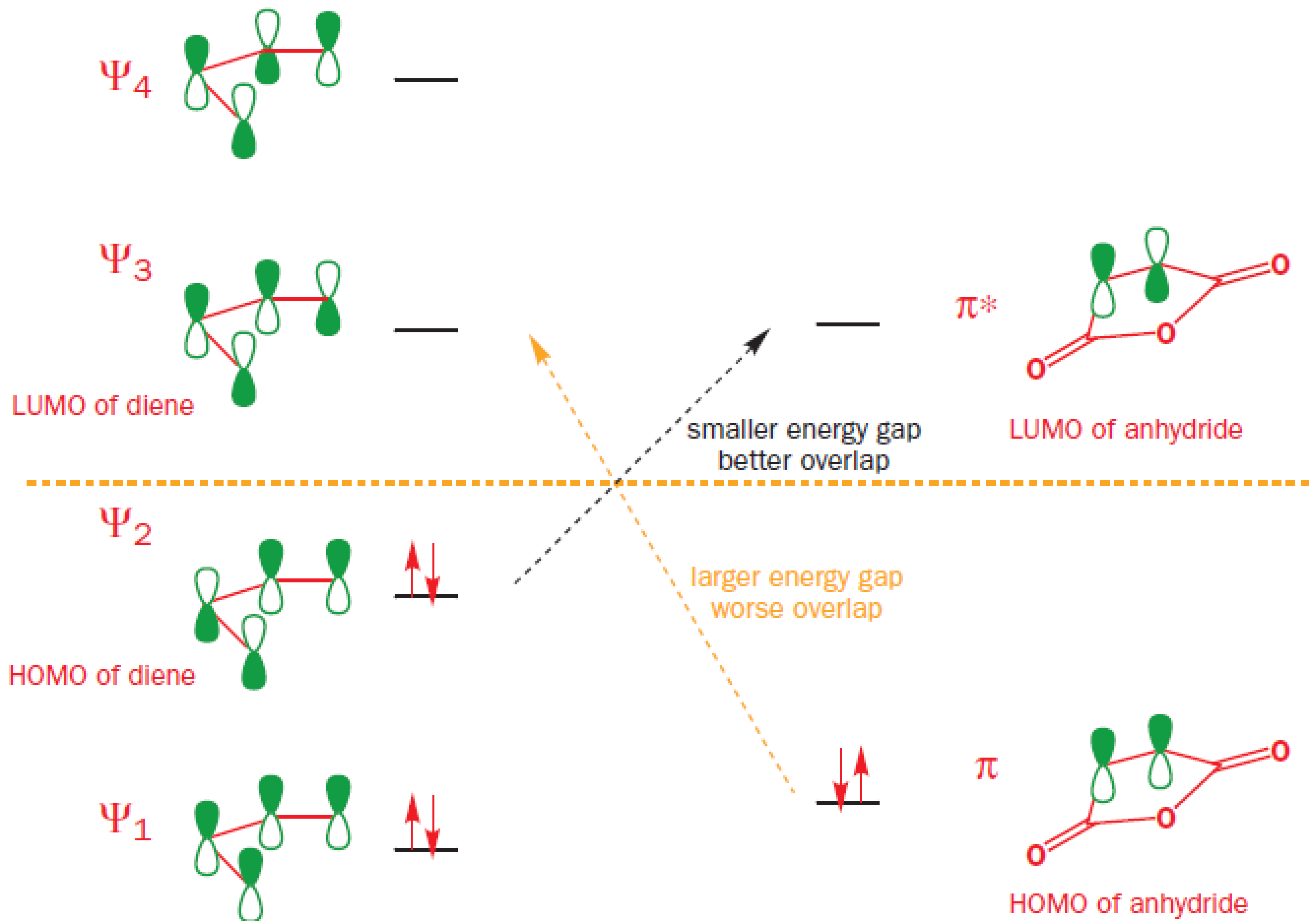


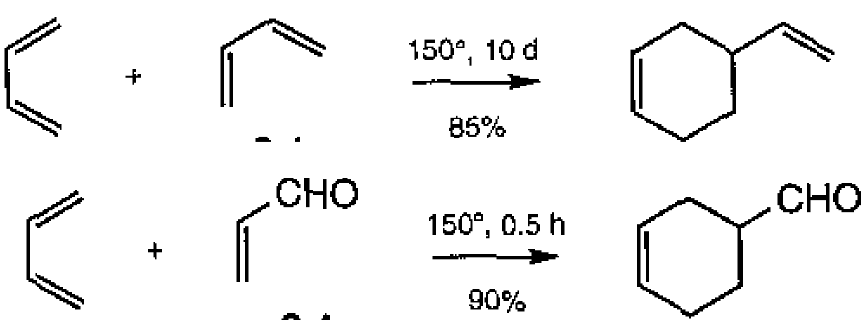


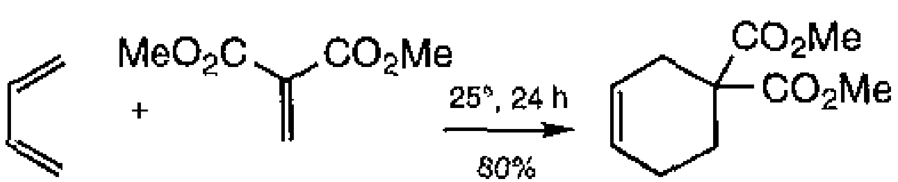


Pericyclic Reactions: Selectivity of Diels-Alder Reaction

Why HOMO of diene interact with the LUMO of Dienophile?







Looking forward

Pericyclic Reaction:

Reactivity and Selectivity of electrocyclic reaction

Pericyclic Reactions in Biological Systems

Course material will be uploaded **after 17:00** h on **every Friday** @

http://www.iitg.ac.in/ckjana/ckjana/Teaching.html