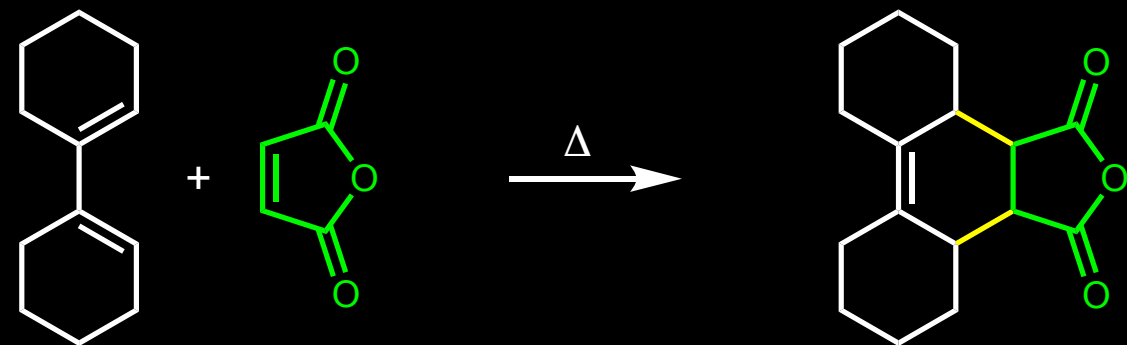
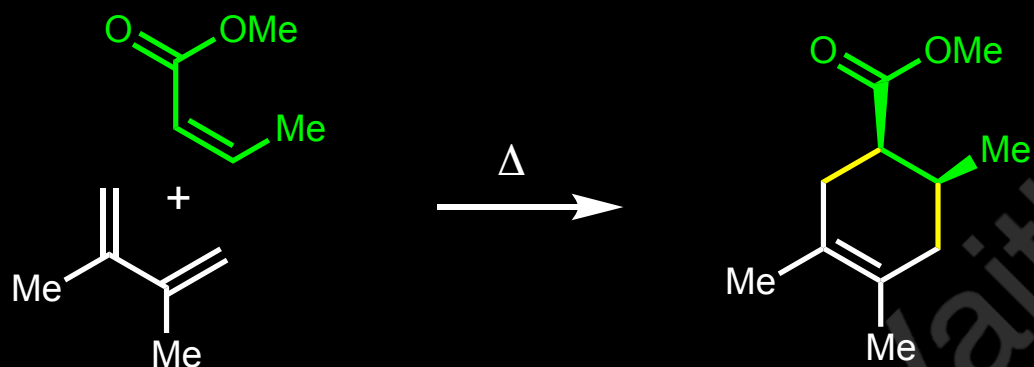
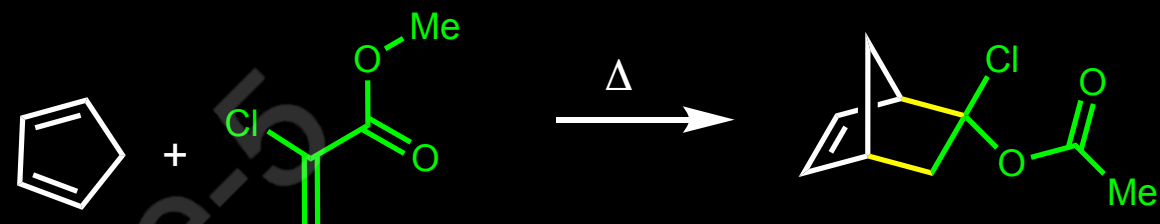
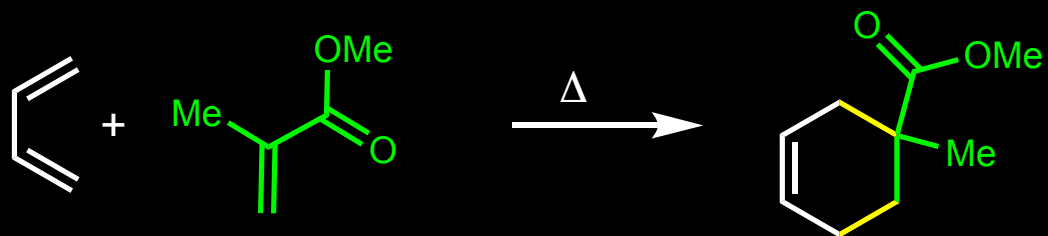


Examples of Diels-Alder Reaction

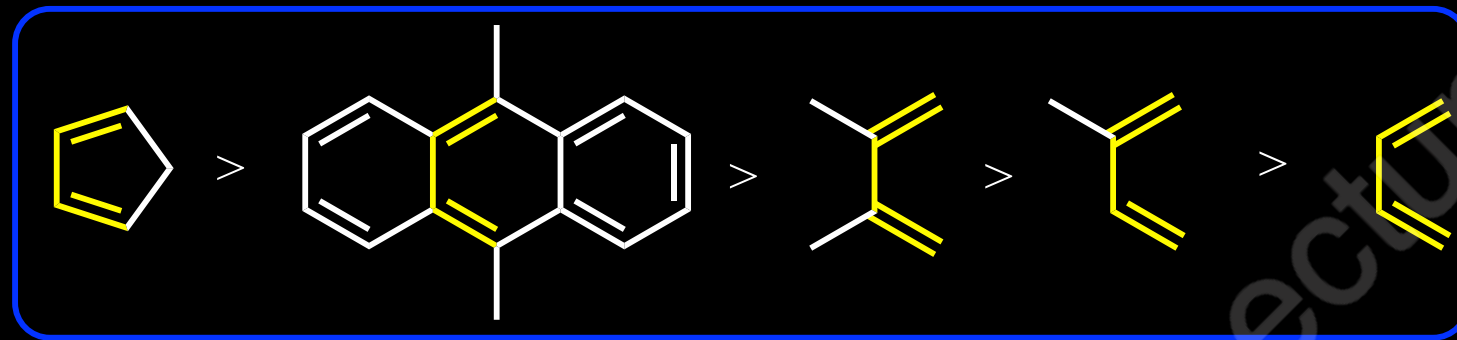


Diels-Alder reaction

Reactivity of Diene

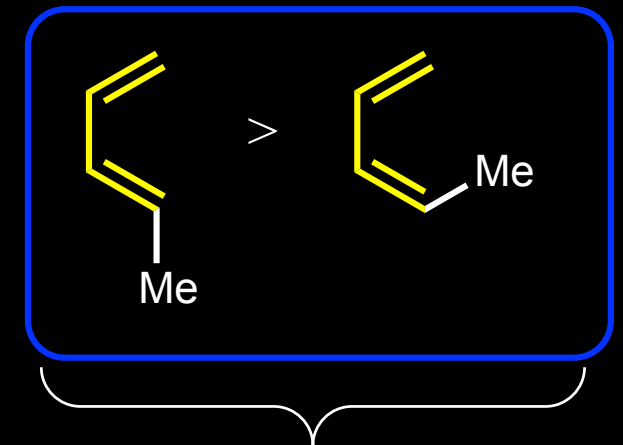
Factors affecting reactivity of diene

- 1) Ability of diene to adopt an *s-Cis* conformation and Planarity of the system
- 2) Electron donor groups



locked in s-Cis conformation

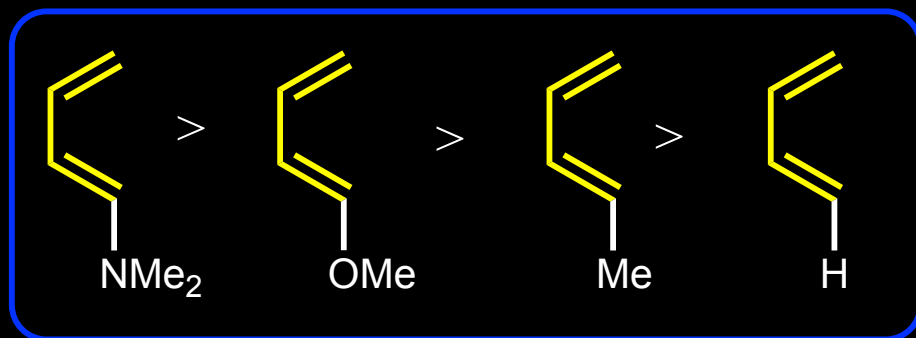
s-Cis and s-Trans conformational stability and also electron donating ability



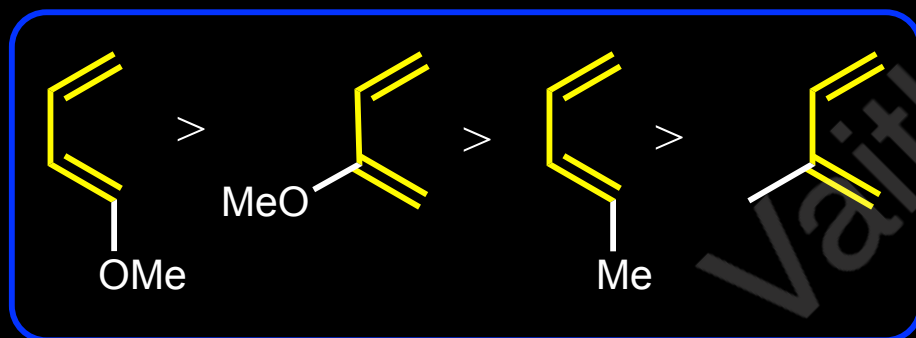
Due to Steric hindrance

Diels-Alder reaction

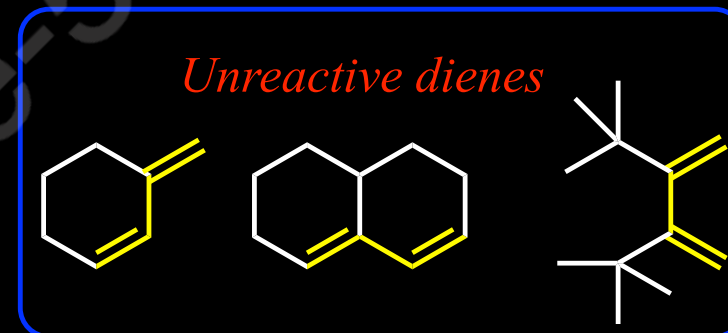
Reactivity of Diene



Higher electron donating tendency



Substituents at position-1 has larger reactivity effect than position-2

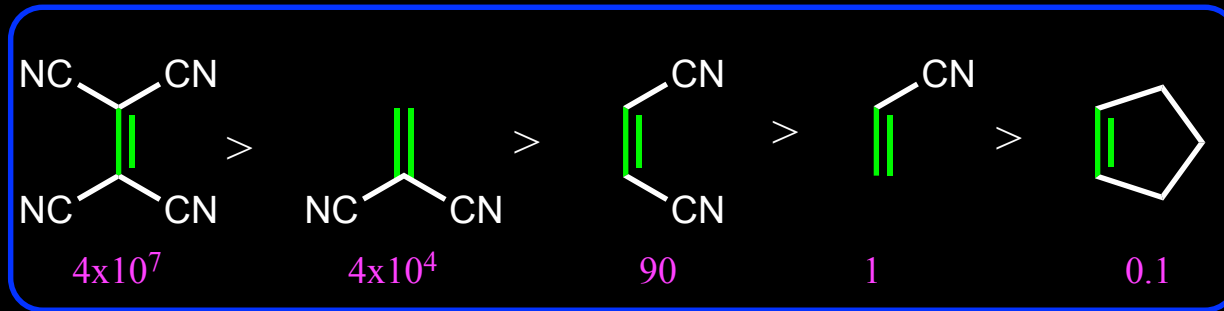


Diels-Alder reaction

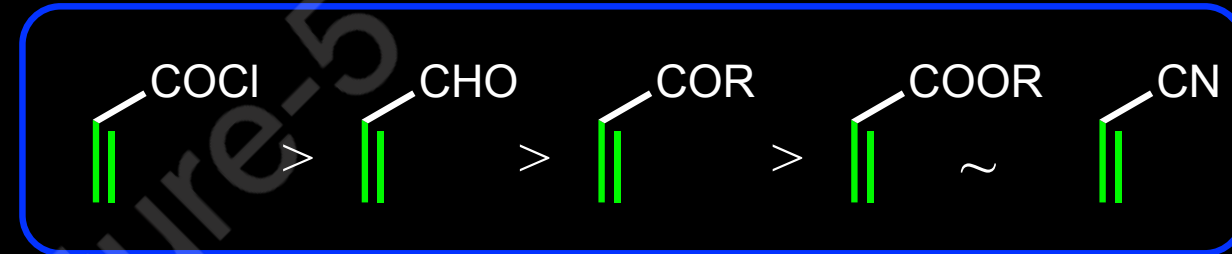
Reactivity of Dienophile

Factors affecting reactivity of dienophile

- 1) Electron withdrawing groups
- 2) A weak π - bond

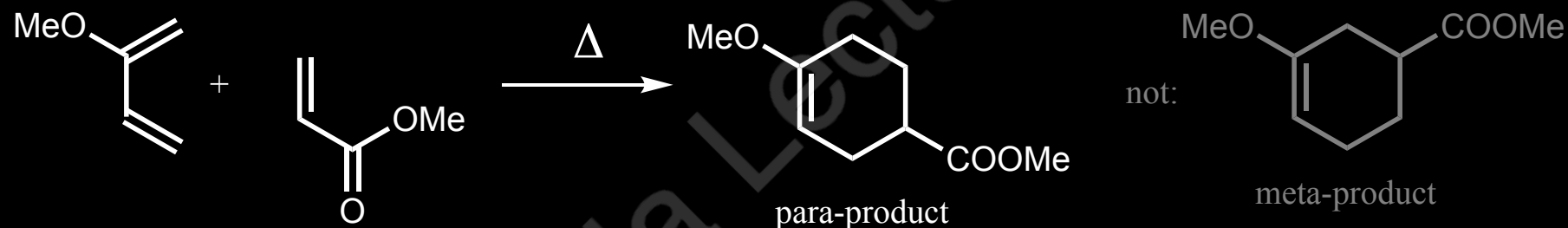
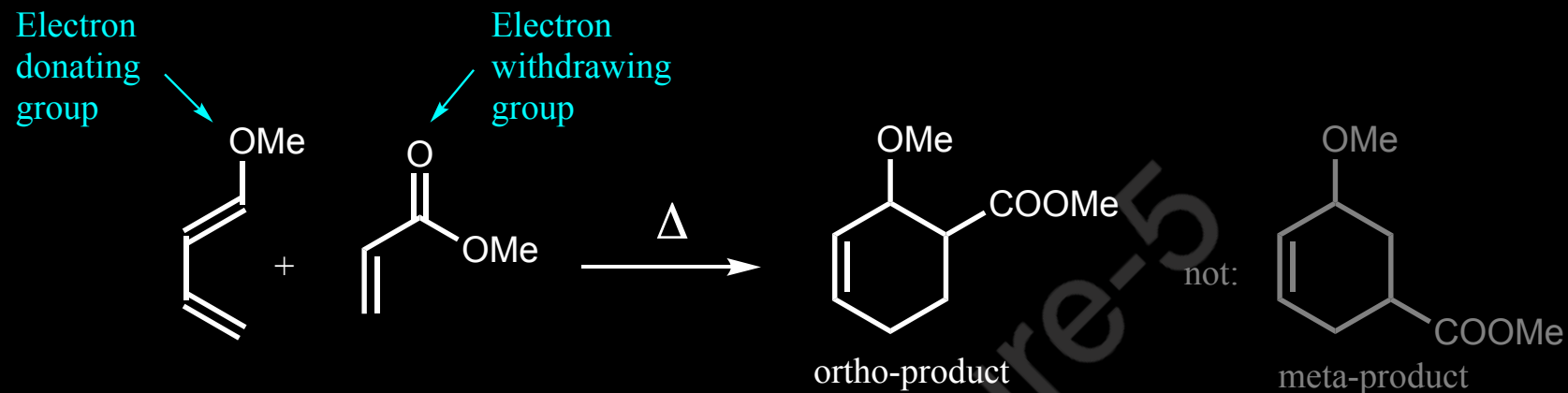


More electron deficiency- higher the reactivity

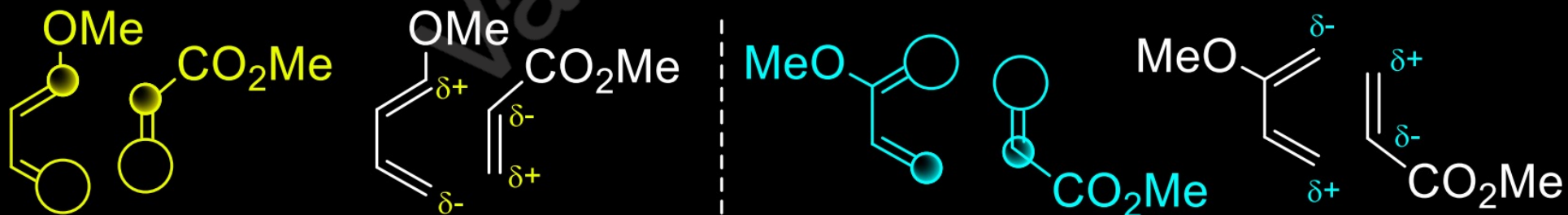


More electron withdrawing tendency- higher the reactivity

Regioselectivity of the Diels-Alder reaction

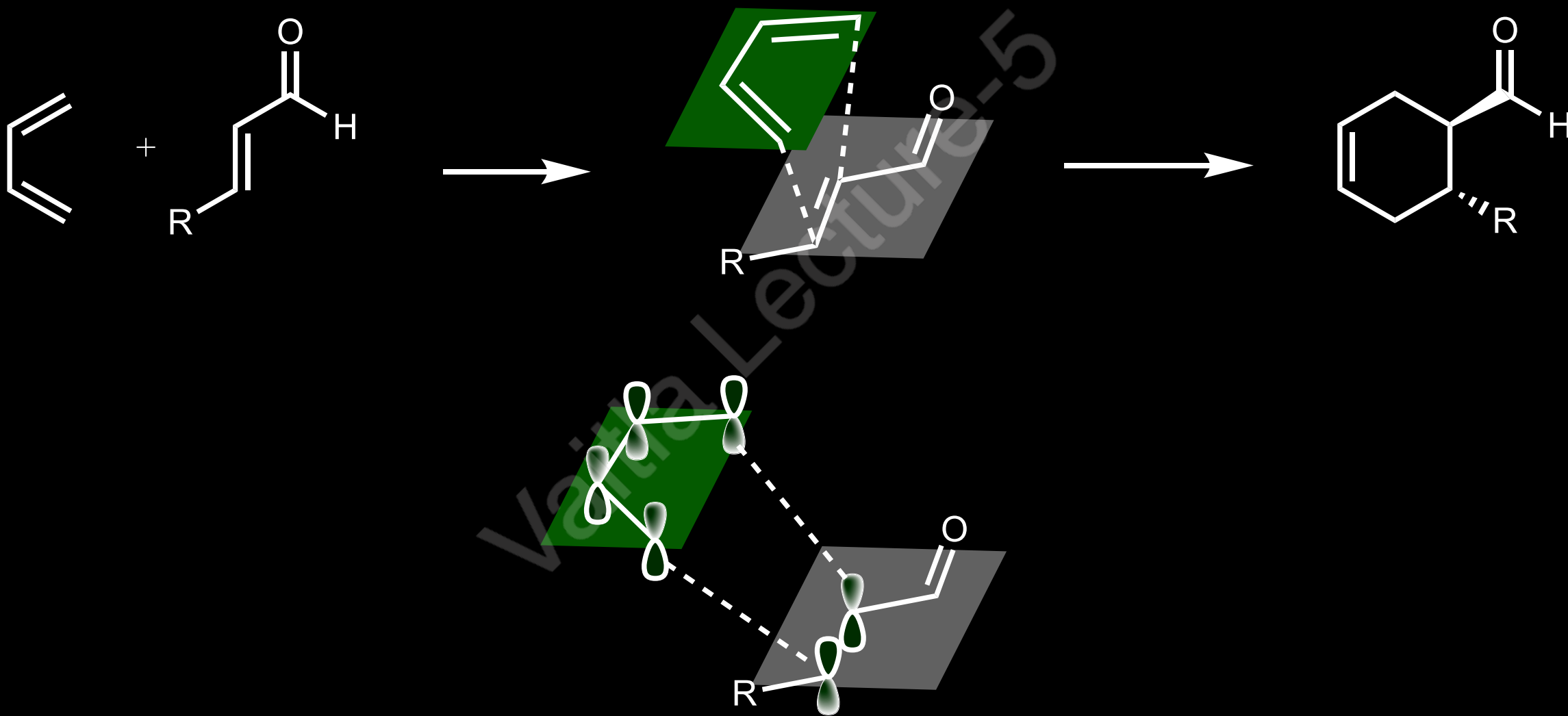


Due to size of MOs, and distribution of partial charges:



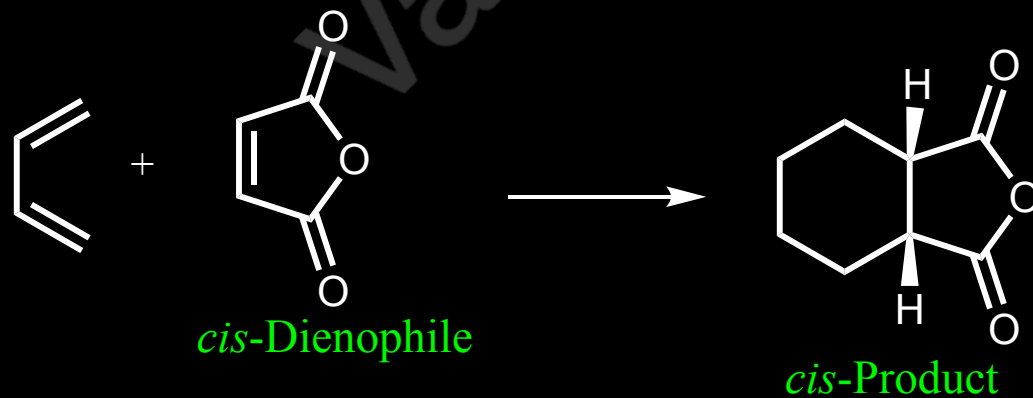
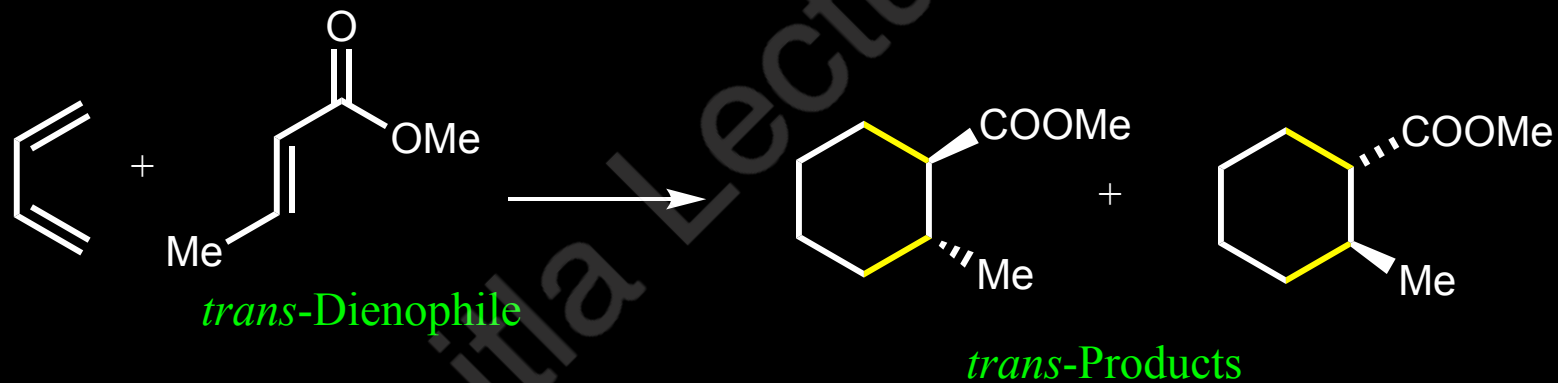
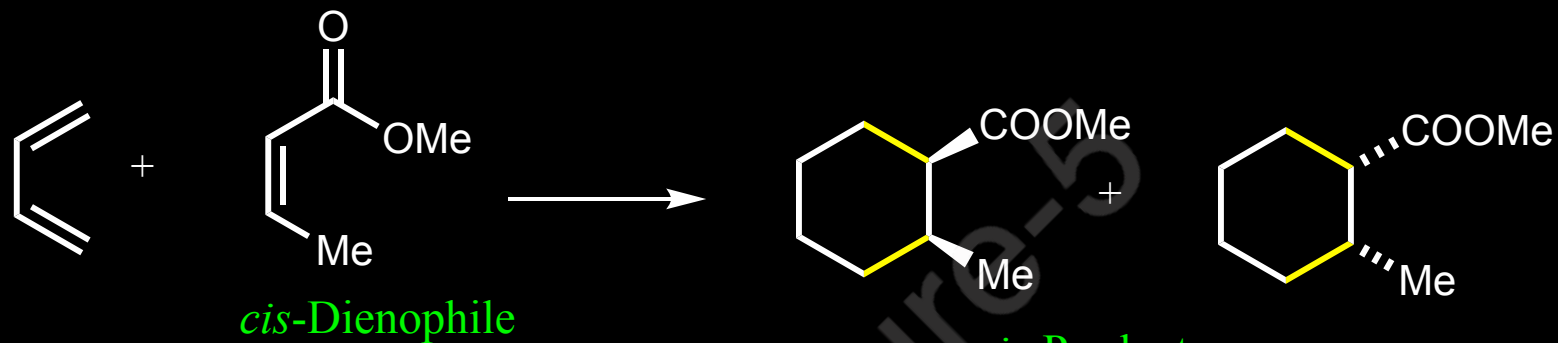
MOs closely matched in size react with each other more efficiently (stepwise analogy).

Stereochemistry of the Diels-Alder reaction

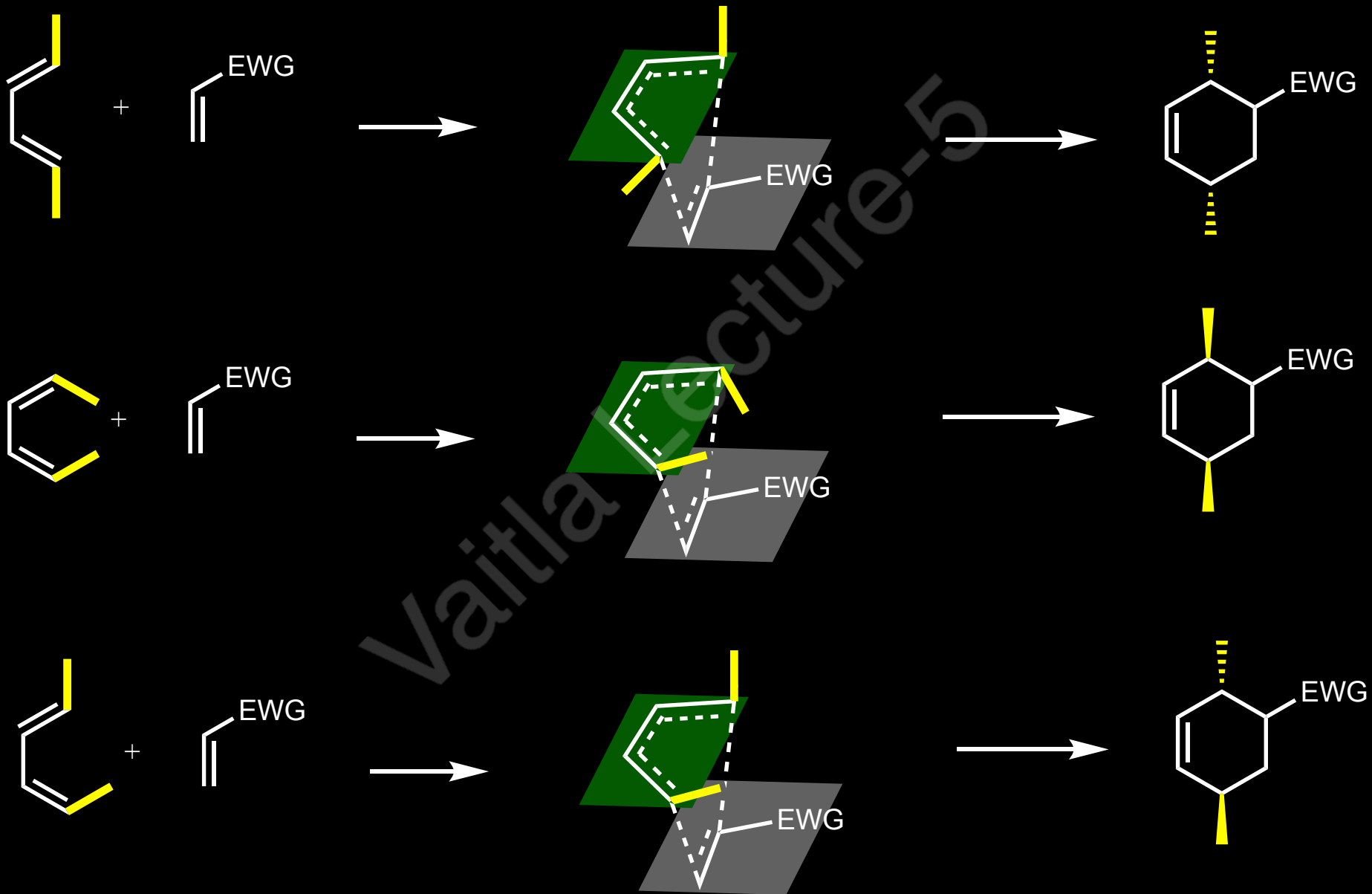


Stereochemistry of the Diels-Alder reaction

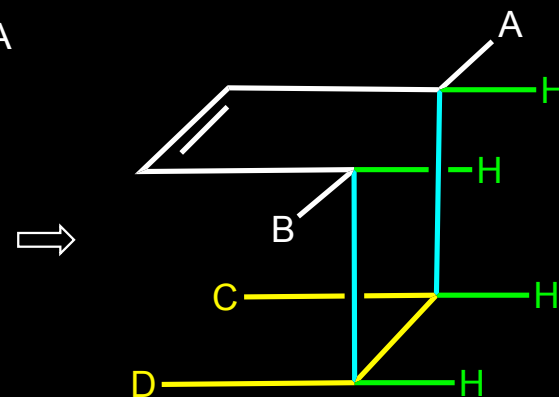
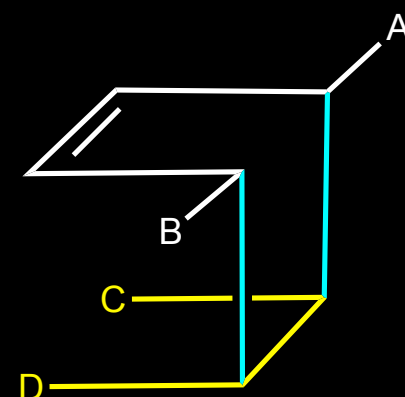
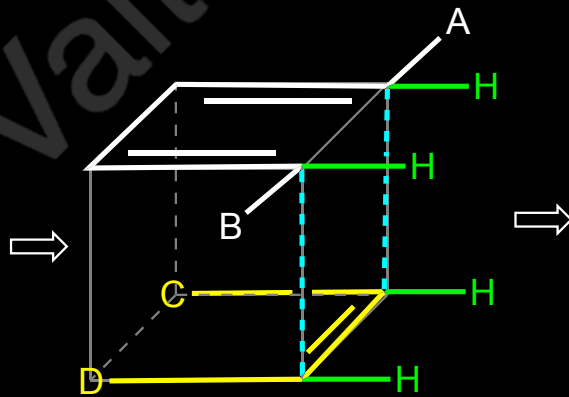
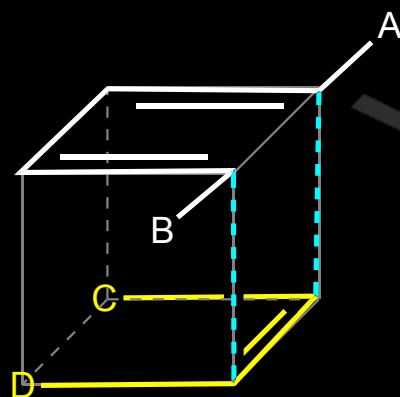
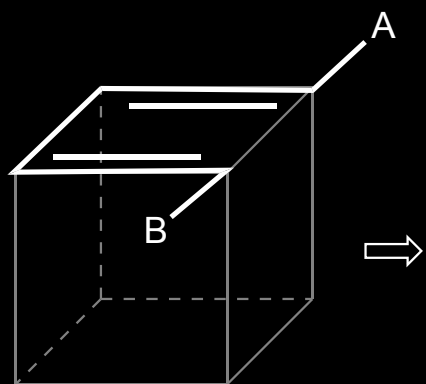
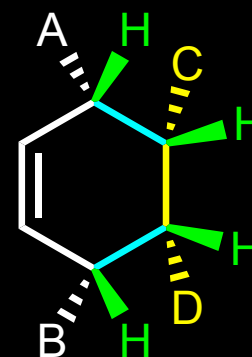
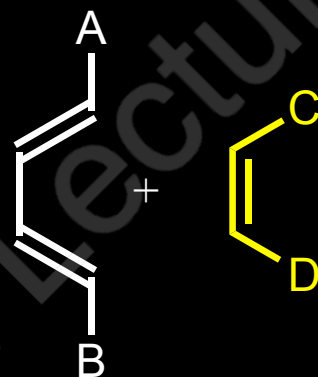
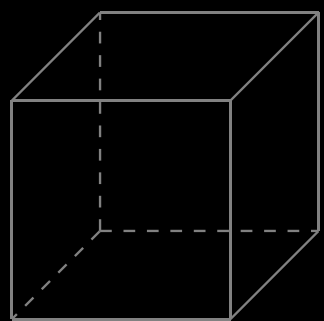
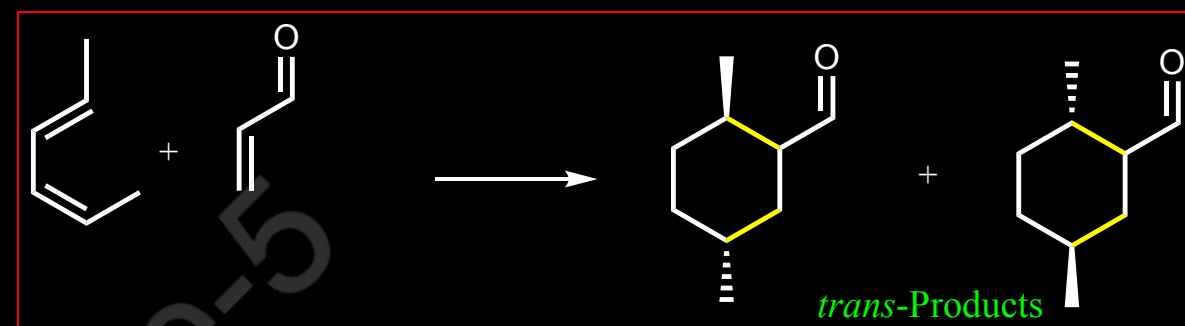
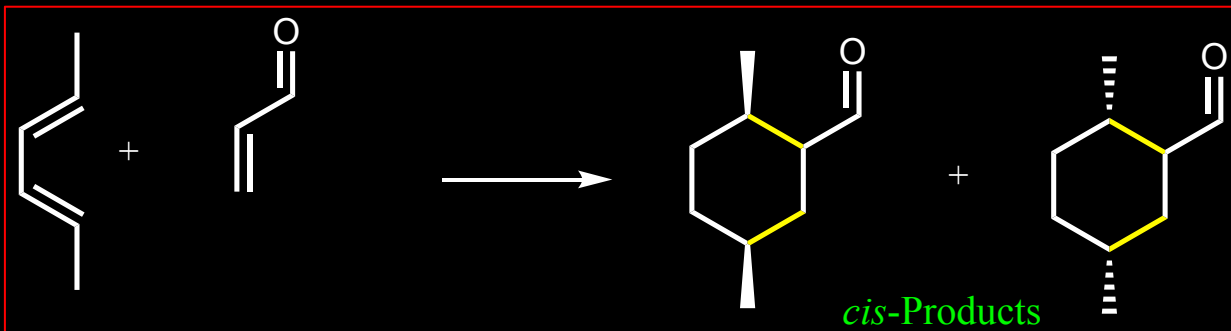
Relative orientation of the groups in the dienophile remains unchanged



Stereochemistry of the Diels-Alder reaction

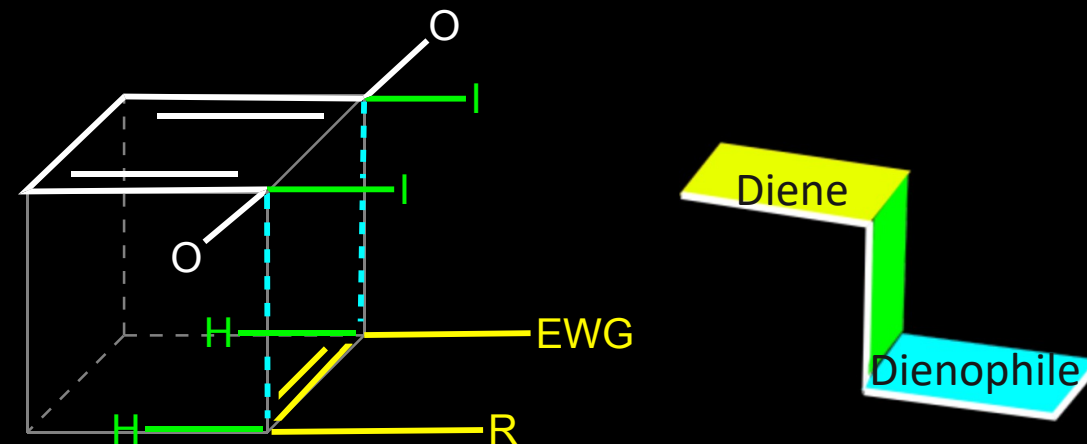
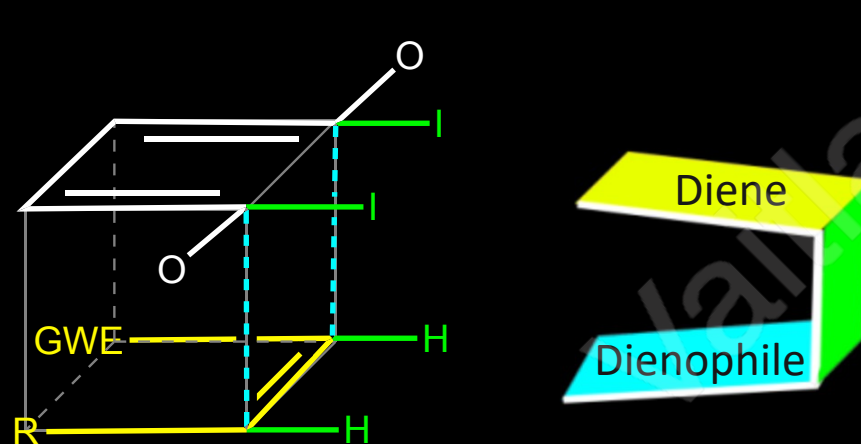
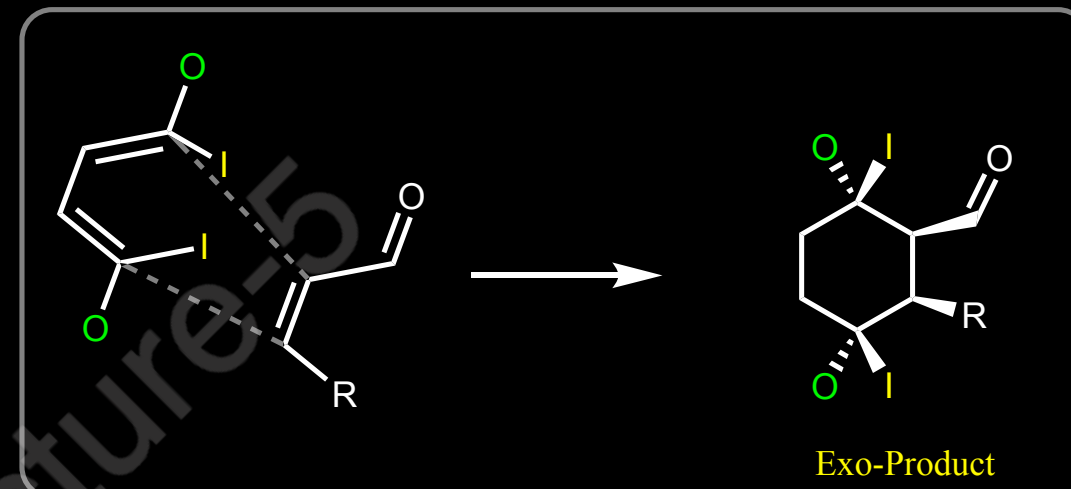
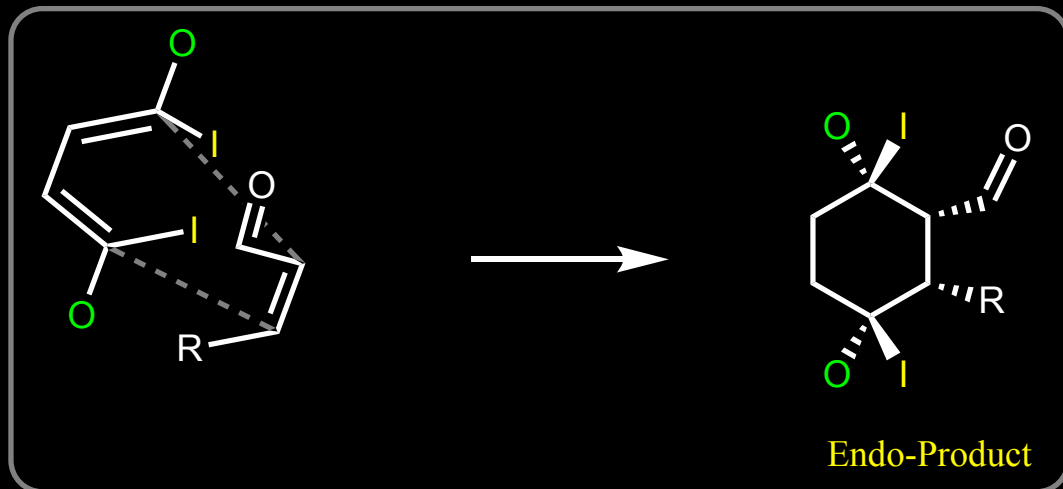


Stereochemistry of the Diels-Alder reaction



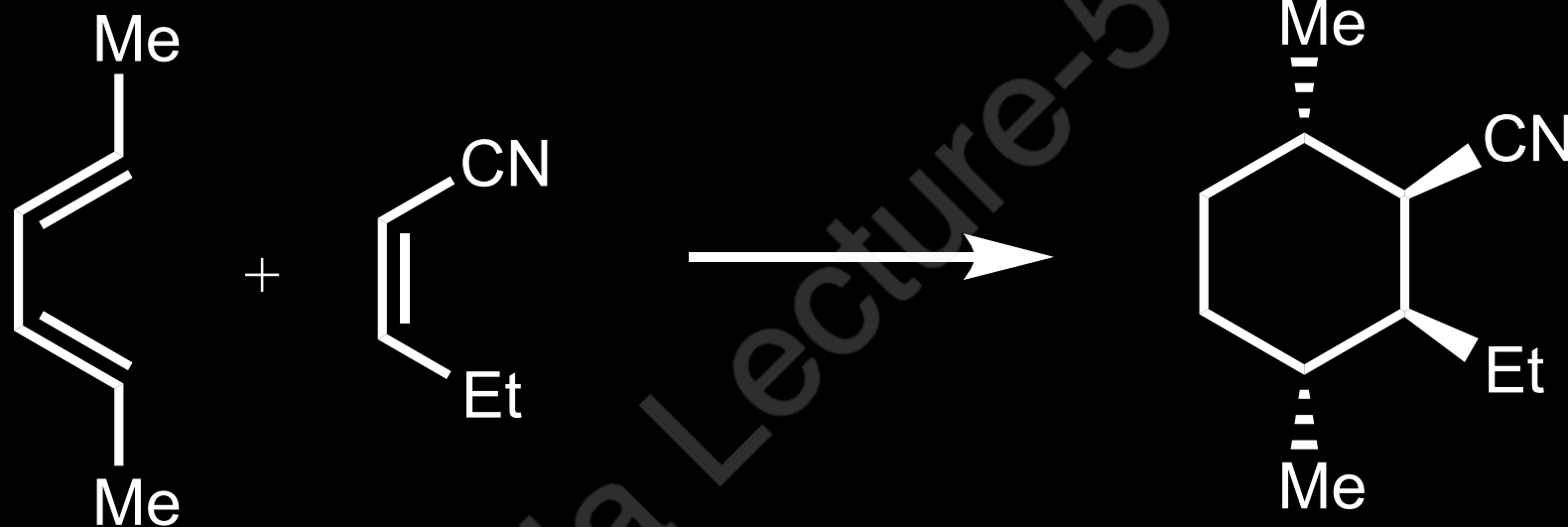
Stereochemistry of the Diels-Alder reaction

Endo and Exo isomers



Endo meaning "within, inner, absorbing, or containing"

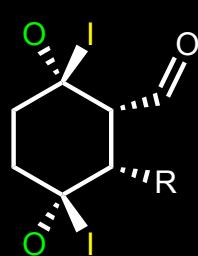
Exo meaning external; from outside.



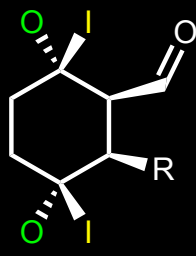
Is it Exo Product
or Endo Product?

Stereochemistry of the Diels-Alder reaction

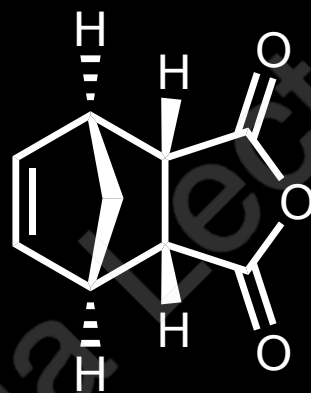
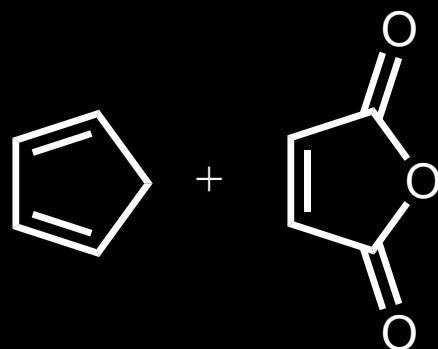
Endo and Exo isomers



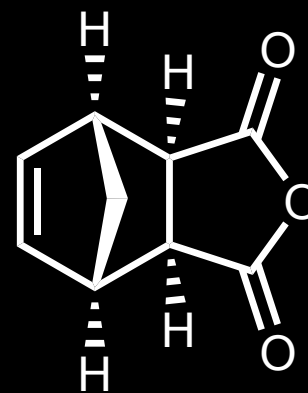
Endo-Product



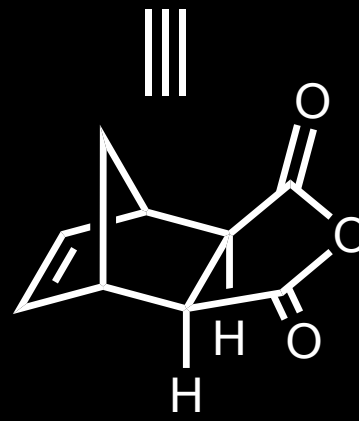
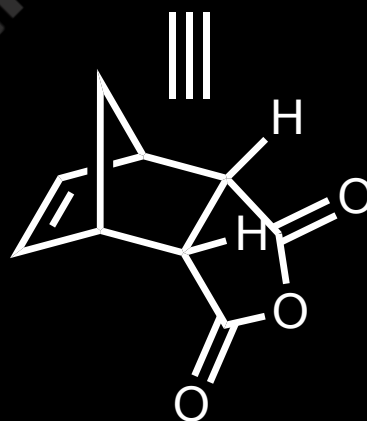
Exo-Product



Endo product

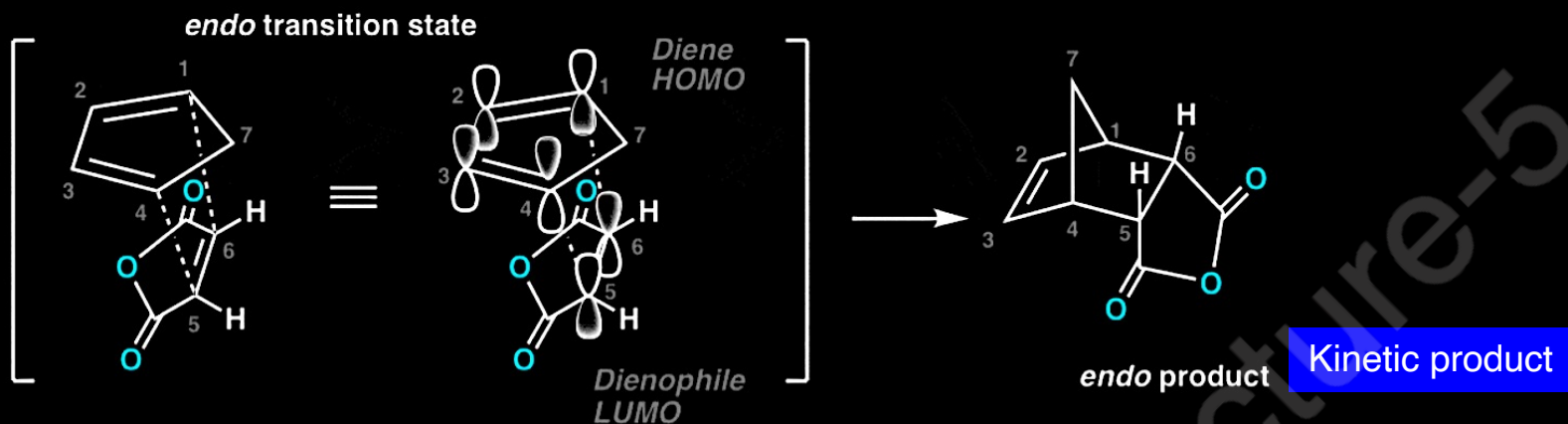


Exo product



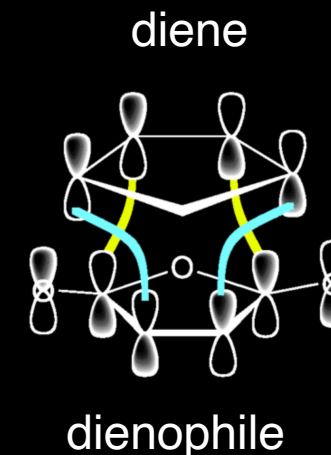
Stereochemistry of the Diels-Alder reaction


exo and endo Transition States and Molecular Orbitals




Interaction between extended π -orbitals of diene and dienophile is possible which can lower the energy of the transition state

Lower –energy transition state = faster rate!



 Bond forming interactions

 Secondary orbital interactions

