Organic Chemistry and the Diels-Alder Reaction

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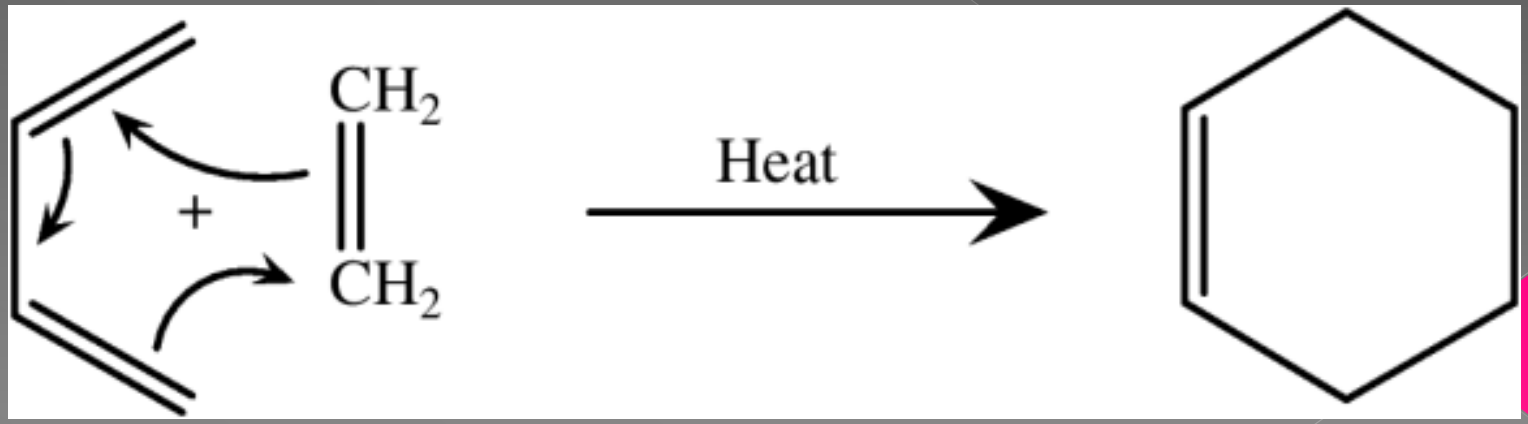
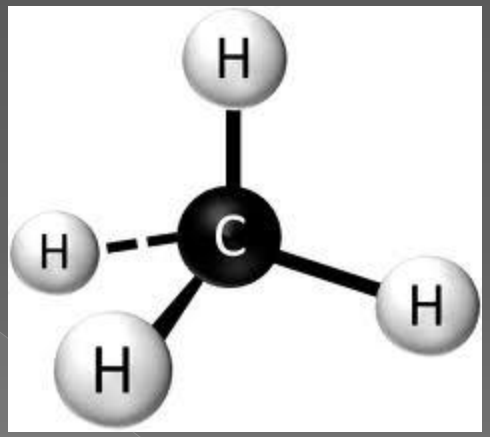
Math 198

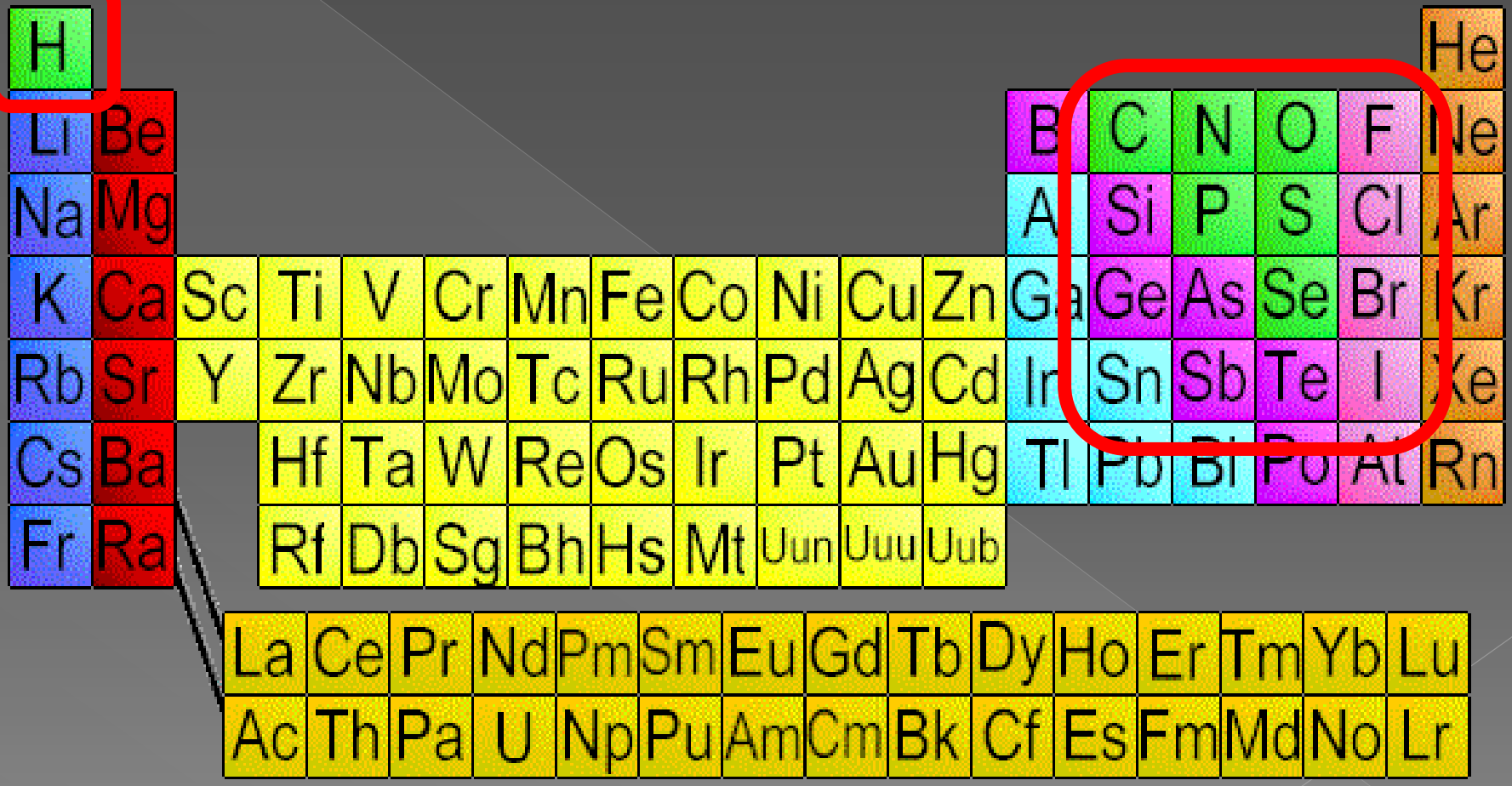


Organic Chemistry Background

- Structure, properties, composition, reactions, and preparation of carbon-based compounds
- May contain other atoms:
  - hydrogen
  - oxygen
  - nitrogen
  - halogens (fluorine, chlorine, bromine, iodine)
  - others too!



Periodic Table!

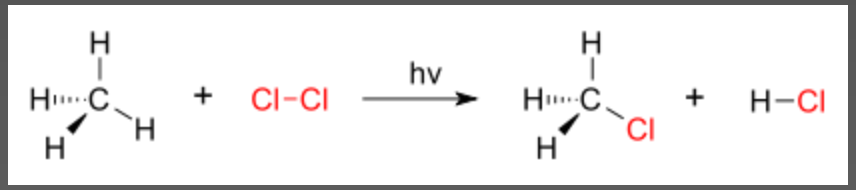


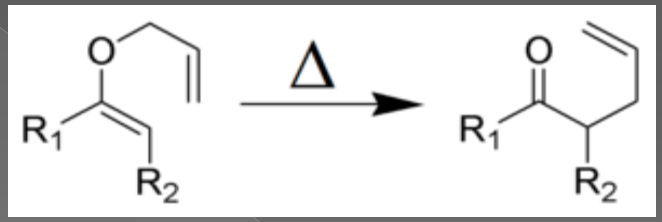
More Background

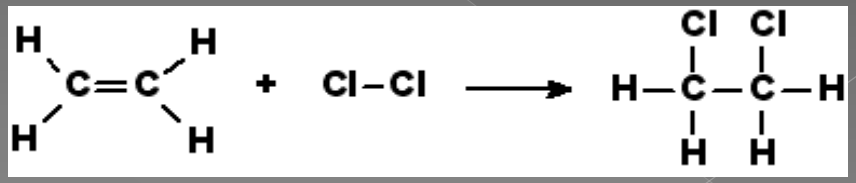
- Range of applications for organic compounds is immense
  - Plastics
  - Drugs (pharmaceuticals and others)
  - Petrochemicals
  - Food
  - Explosives
  - Paint
  - More!

Organic Reactions

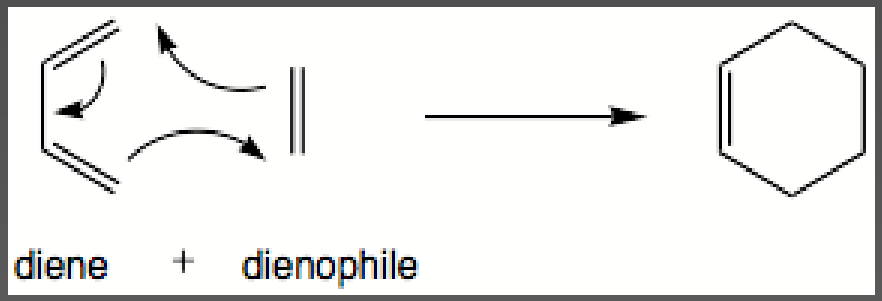
- Basic reactions:
  - Addition
  - Substitution
  - Elimination
  - Rearrangement
  - Photochemical
  - Redox





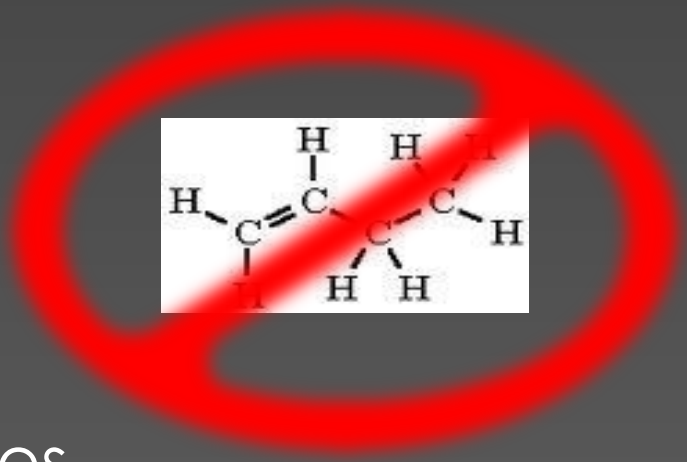


Diels-Alder Reaction

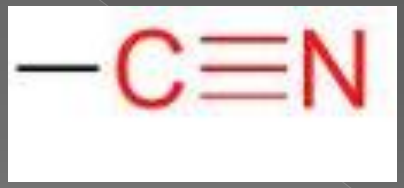


- Addition reaction
  - cycloaddition
  - pericyclic
- Reaction between a **diene** and a **dienophile** to form a substituted **cyclohexene**
  - **diene**: hydrocarbon that contains two double bonds
  - **dienophile**: unsaturated hydrocarbon, has at least one C=C double bond
  - **cyclohexene**: six membered carbon ring with one C=C double bond

Requirements



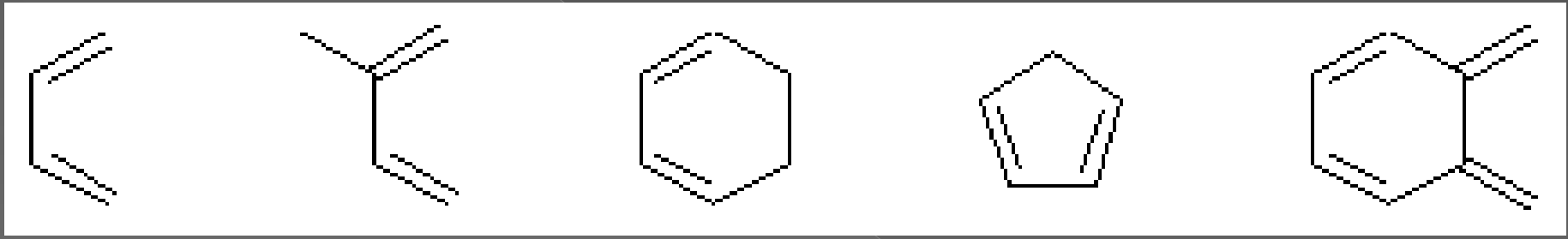
- Good dienophile
  - Not simple alkenes or alkynes
  - One or more electron-withdrawing carbonyl groups (oxygen) or cyano groups (nitrogen)



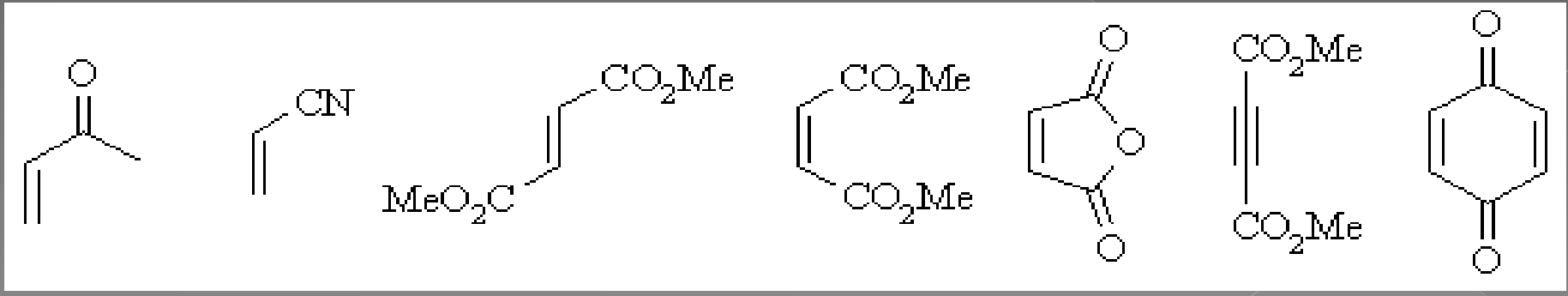
  - These groups pull electron density away from the C=C double bond, making it more likely to react.

Dienes and Dienophiles

- Good dienes:

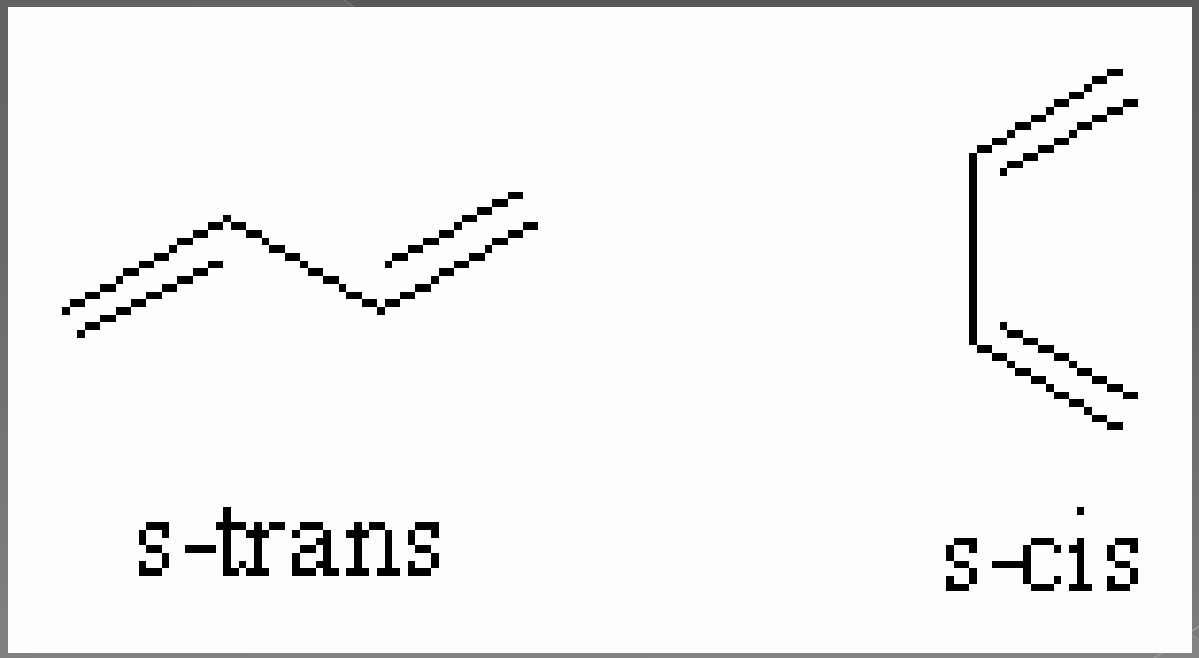


- Good dienophiles:



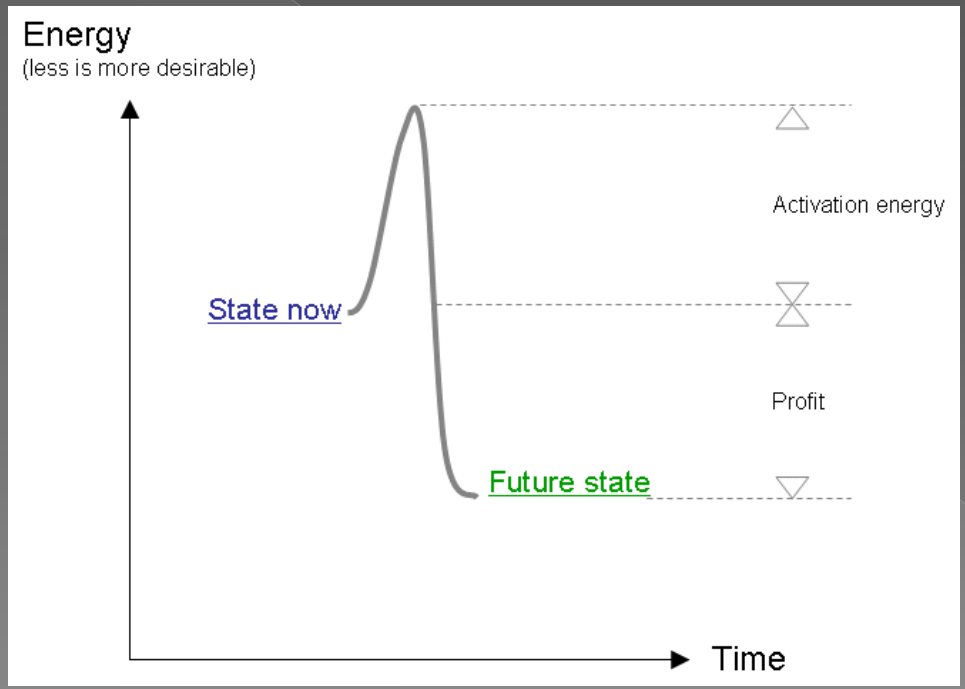
Reaction Continued

- Conformation of **diene**: needs to be s-cis NOT s-trans



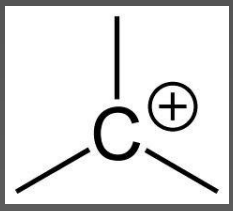
More Requirements

- Heat! Reaction can't run without an initial push to overcome the activation energy

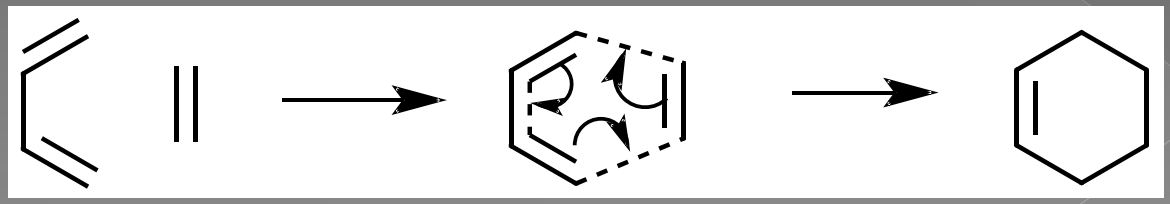


What is a pericyclic reaction anyways?

- Most organic reactions go through a *transition state* where a *carbocation intermediate* is formed



- A pericyclic reaction occurs when there is NO intermediate formed. The reaction progresses in a *concerted* fashion, and the result is a cyclic molecule.

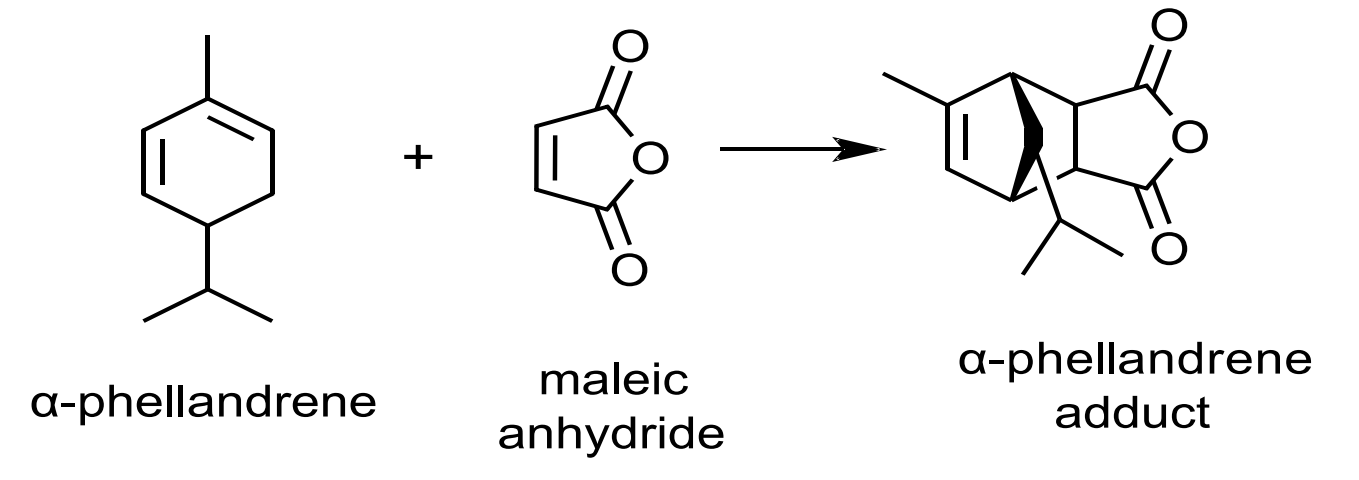


More about Diels-Alder!

- Otto Paul Hermann Diels and Kurt Alder first documented the reaction in 1928
- They were awarded the Nobel Prize in Chemistry in 1950 for their work on the new reaction.
- Generally considered one of the more useful reactions in organic chemistry since it requires very little energy to create a *cyclohexene ring*, which is useful in many other organic reactions.

Example: Eucalyptus Oil

- The Diels-Alder reaction is used to create the active ingredient in synthetic *Eucalyptus dives* oil, which is used in Bengay and similar products

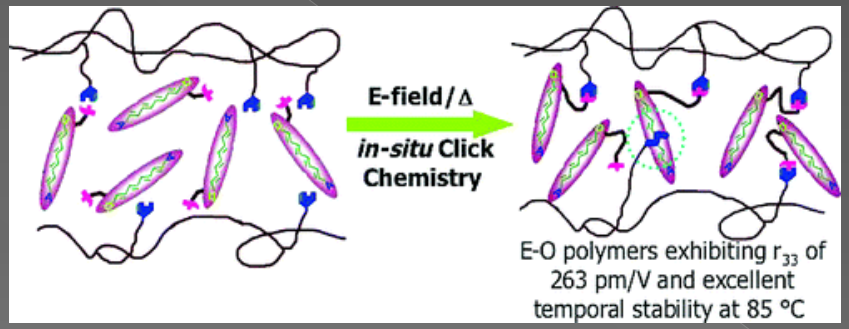


Interesting Fact!

- Interestingly, many Diels-Alder reactions occur much faster in water than in organic solvents. Scientists are still working on finding out why aqueous environment accelerates this reaction.

Use of Diels-Alder

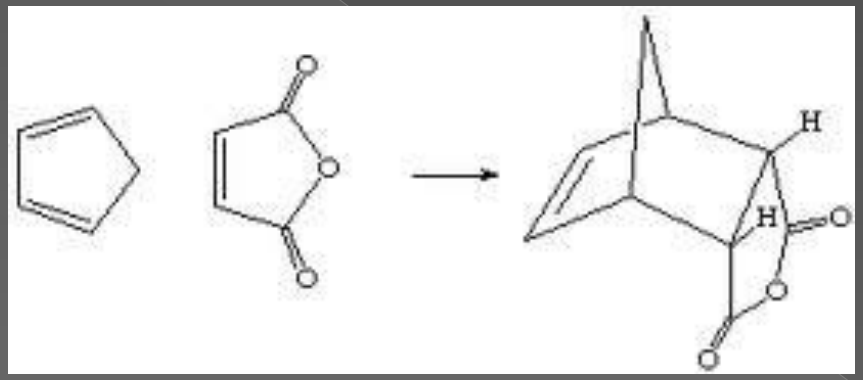
- Incorporating Highly Efficient Polyenic Chromophores into Maleimide-Containing Side-Chain Polymers for Electro-Optics

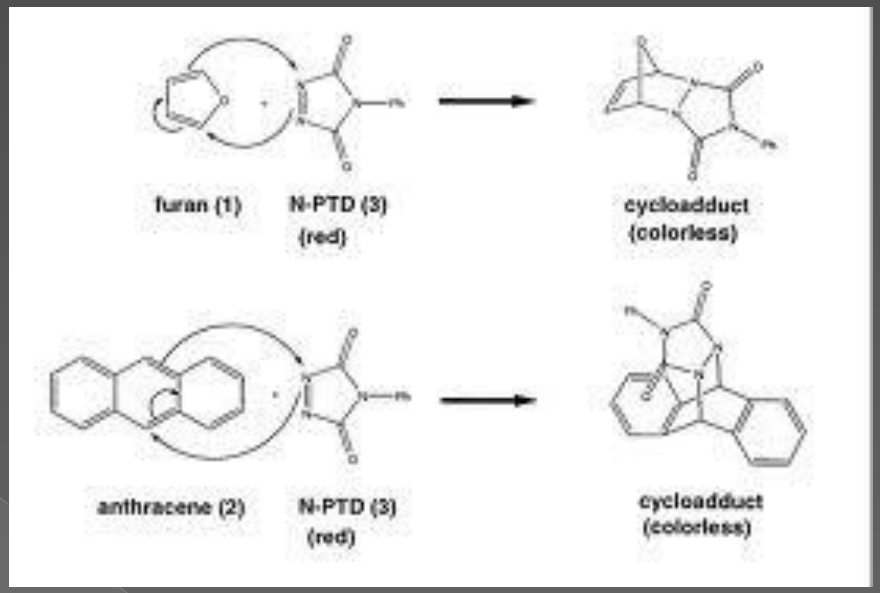


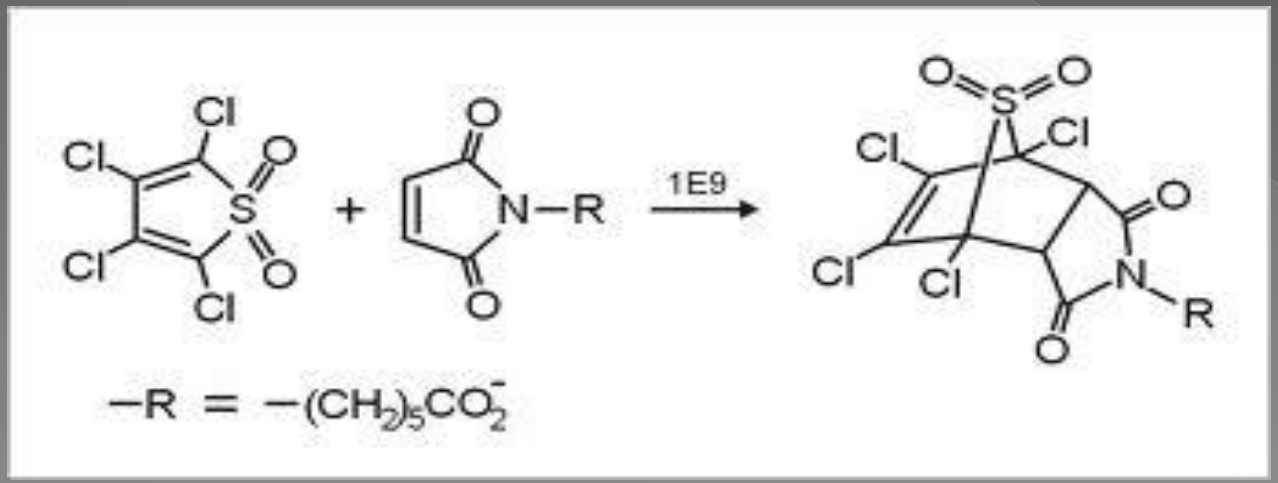
http://pubs.acs.org/doi/abs/10.1021/ma802612g

- Enzyme-catalyzed biosynthesis of a fungal metabolite
- Conducting polymers

More Examples







Sources

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