Diels-Alder reaction

Learning outcome

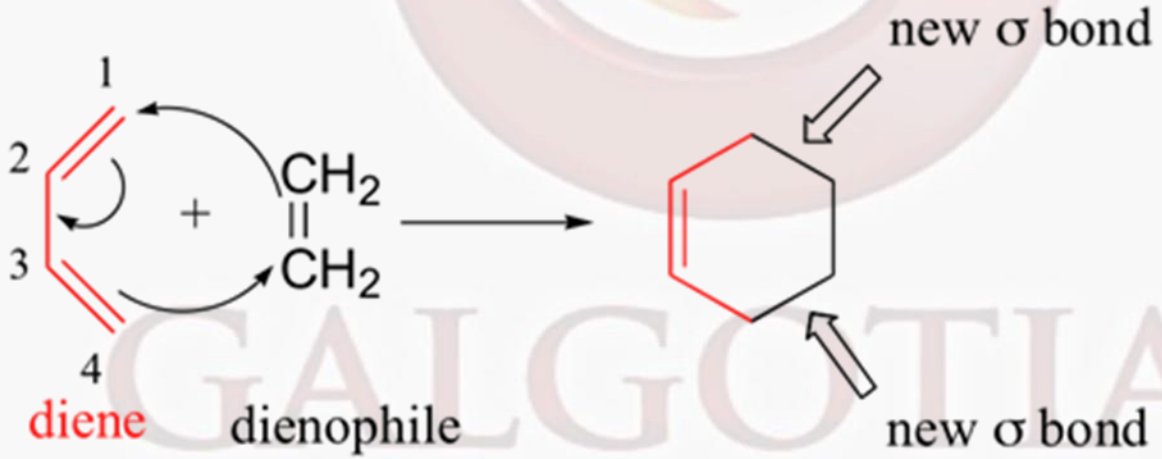
After studying this lecture, you shall be able to:

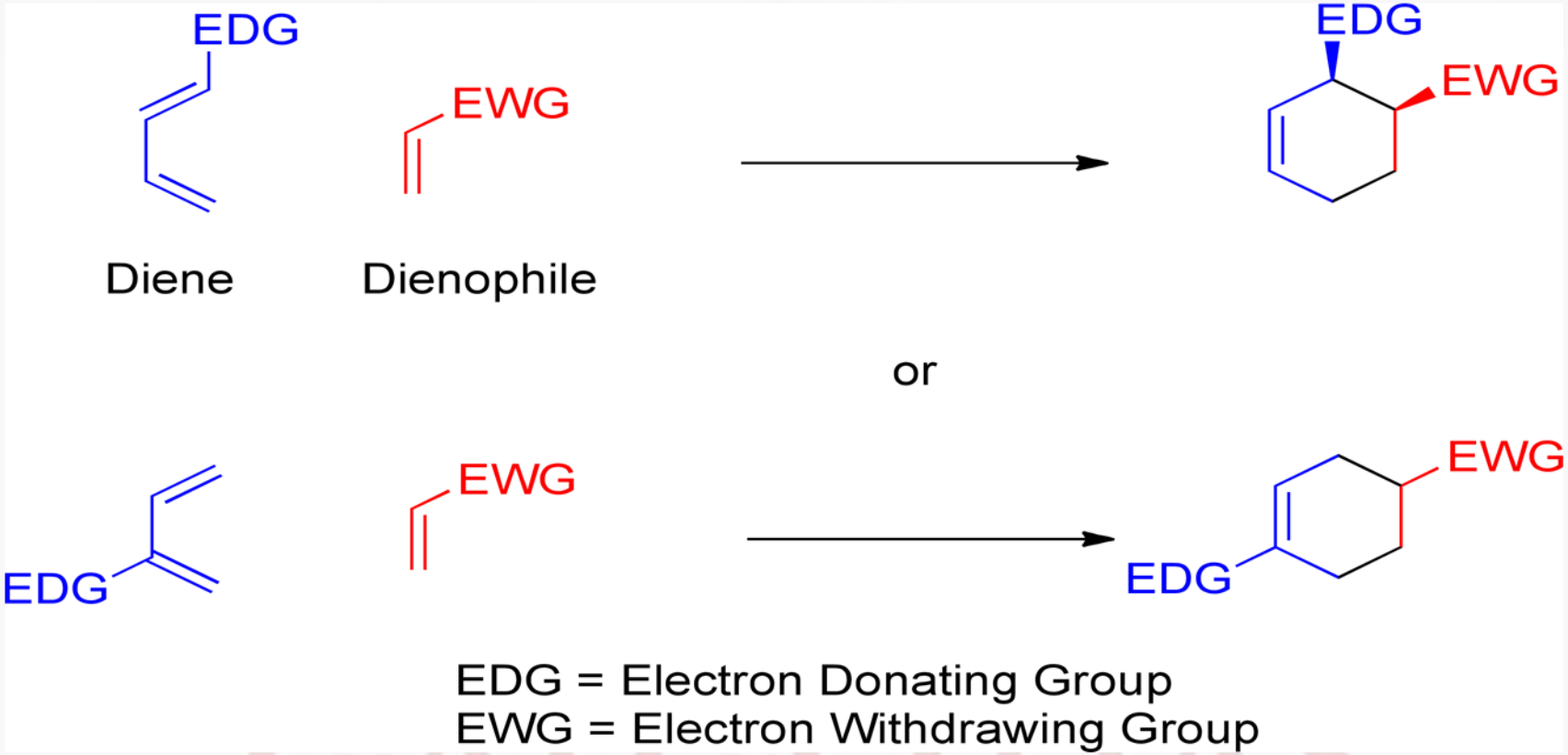
- Explain of substituents on orientation
- Explain of substituents on reactivity
- Explain electronic interpretation of ortho and para directive influence on groups

Diels- Alder reaction

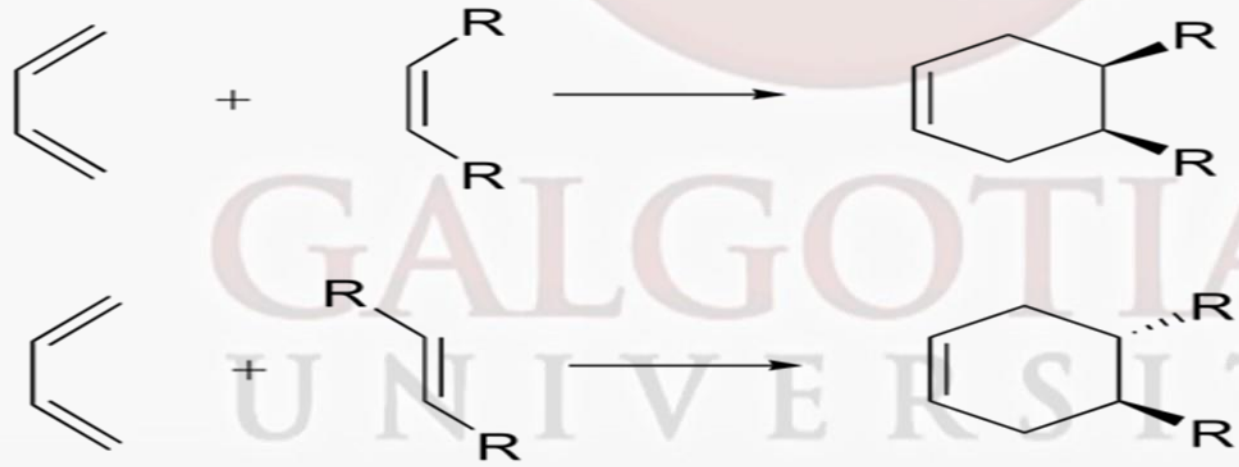
- The Diels-Alder reaction is an organic reaction that is used to convert a conjugated diene (a molecule with two alternating double bonds) and a dienophile (an alkene) to a cyclic olefin.
- This process is concerted, where bonds form and break at the same time, and the entire reaction takes place in one step in the presence of heat.
- The class of reactions to which Diels-Alder belong is termed as cycloaddition.

- The electrons are transferred cyclically between the diene and the alkene to form a cyclic adduct. Diels-Alder reactions are stereospecific.
- The substituents attached to both the diene and the dienophile and retain their stereochemistry throughout the reaction.
- Electron withdrawing groups on the dienophile and electron-donating group on the diene facilitate reaction



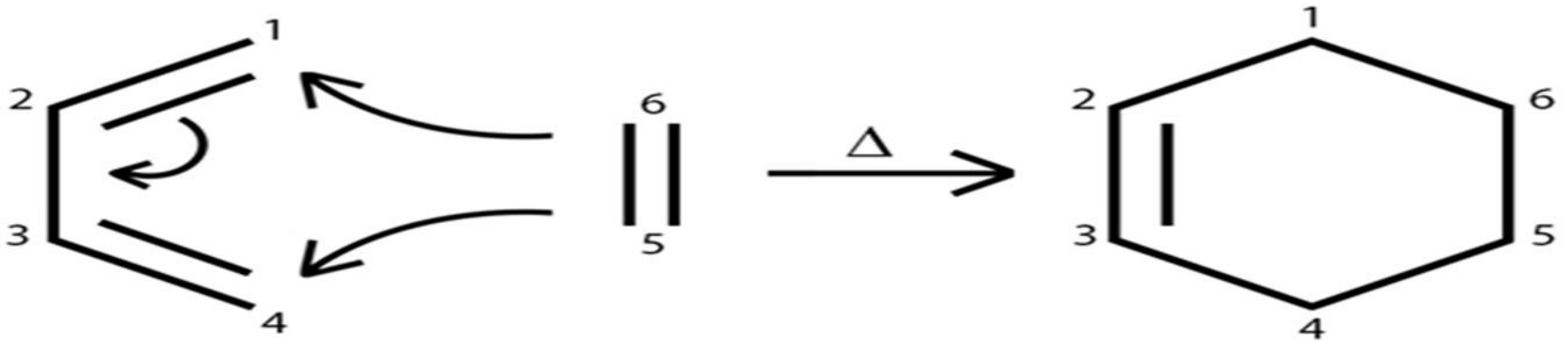

EDG
EWG
EDG
EWG
Diene
Dienophile
or
EDG
EWG
EWG
EDG
EDG = Electron Donating Group
EWG = Electron Withdrawing Group

- In a Diels-Alder reaction, the alkene reacting partner is referred to as the **dienophile**.
- Essentially, this process involves overlap of the 2p orbitals on carbons 1 and 4 of the diene with 2p orbitals on the two sp^2-hybridized carbons of the dienophile.
- Both of these new overlaps end up forming new sigma bonds, and a new pi bond is formed between carbon 2 and 3 of the diene.
- The Diels-Alder reaction is enormously useful for synthetic organic chemists, not only because ring-forming reactions are useful in general but also because in many cases two new stereocenters are formed, and the reaction is inherently stereospecific. A cis dienophile will generate a ring with cis substitution, while a trans dienophile will generate a ring with trans substitution:



Mechanism of Diels-Alder Reaction

1. Electrons from the dienophile attack carbon (C) 1 on the diene resulting in a single bond between C1 and C6.
2. Electrons from the double bond between C1 and C2 relocates to between C2 and C3.
3. Double bond between C3 and C4 are broken and the electrons form a single bond between C4 and C5 to form the product.
4. All processes take place in a single step.



Diene (Butadiene) | Dienophile (Ethylene) | Cyclic adduct (Cyclohexene)

References:

1. Morrison, R. N. & Boyd, R. N. *Organic Chemistry*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
2. Finar, I. L. *Organic Chemistry (Volume 1)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education).
3. Finar, I. L. *Organic Chemistry (Volume 2: Stereochemistry and the Chemistry ofNatural Products)*, Dorling Kindersley (India) Pvt. Ltd. (Pearson Education.
4. Eliel, E. L. & Wilen, S. H. *Stereochemistry of Organic Compounds*, Wiley: London, 1994.
5. Kalsi, P. S. *Stereochemistry Conformation and Mechanism*, New Age International, 2005.
6. McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning India Edition, 2013.
7. https://www.chemistrylearner.com/diels-alder-reaction.html
8. https://courses.lumenlearning.com/suny-potsdam-organicchemistry2/chapter/13-3-diels-alder-reaction/
9. https://sites.science.oregonstate.edu/~gablek/CH335/Chapter14/DielsAlder.htm

Thank You