B.Sc. Semester-VI GroupA / DSE-4 Organic Synthesis



# II. Pericyclic Reactions 6. Diels-Alder Reaction



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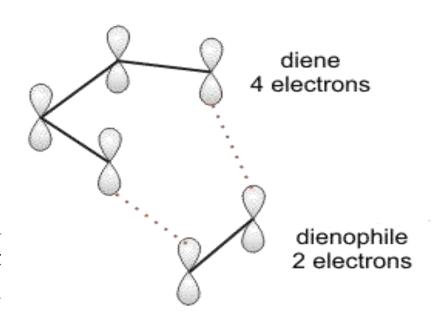
#### **Cycloaddition Reaction**

A **cycloaddition** is a reaction, in which two  $\pi$  bonds are lost and two  $\sigma$  bonds are gained. The resulting reaction is a cyclization reaction.

### 4+2 Cycloaddition Reaction (Supra-Supra)

The Diels-Alder reaction represents the prototype of cycloadditions. Besides the Grignard reaction, it is the most cited name reaction in chemical literature.

The reaction principle was discovered in 1928 by **Otto Diels** and his student **Kurt Alder**. Both were honored with the Nobel Prize for Chemistry in 1950.





**Otto Diels** 1876-1954

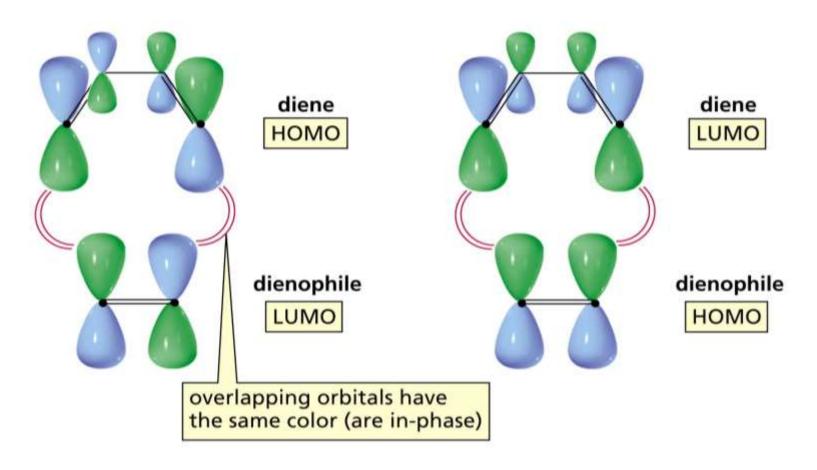


Kurt Alder 1902-1958

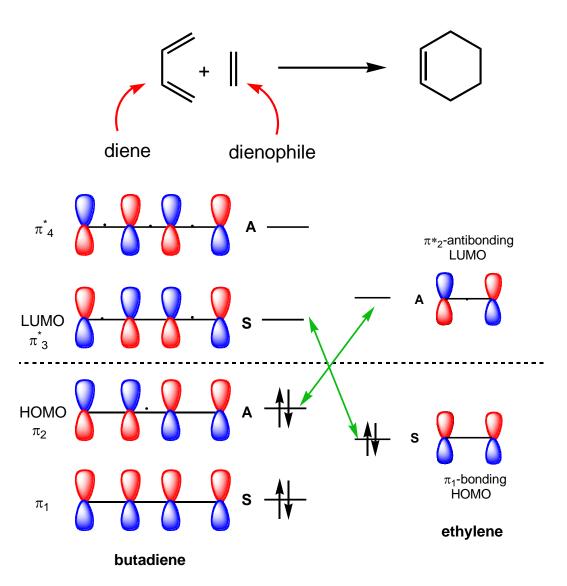
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## Diels-Alder Cycloaddition : Frontier Orbital Intractions 6-e, 4+2 Supra-supra



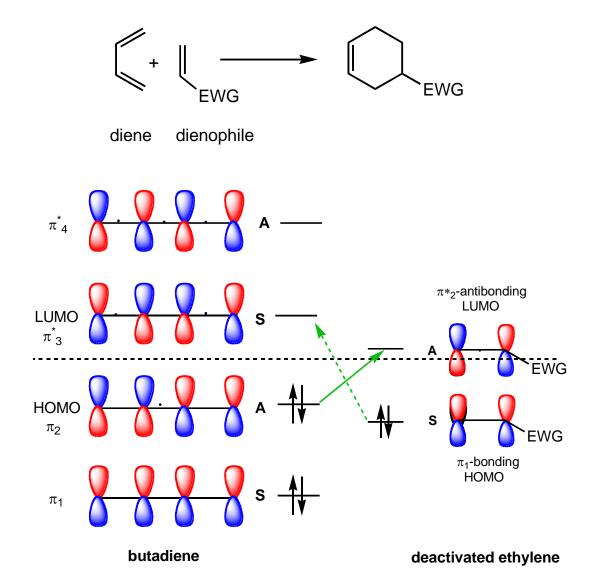
### Diels-Alder Reaction An Allowed [4+2] Cycloaddition



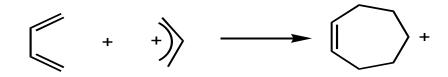
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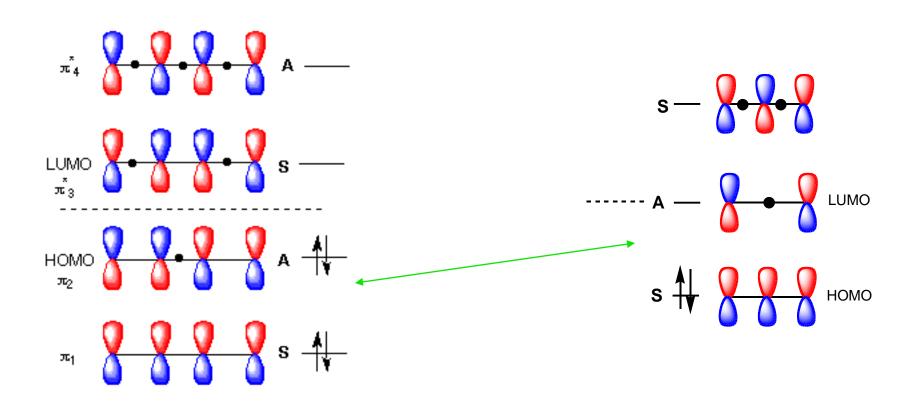
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### Diels-Alder Reaction: The Effect of Electron Withdrawing Groups

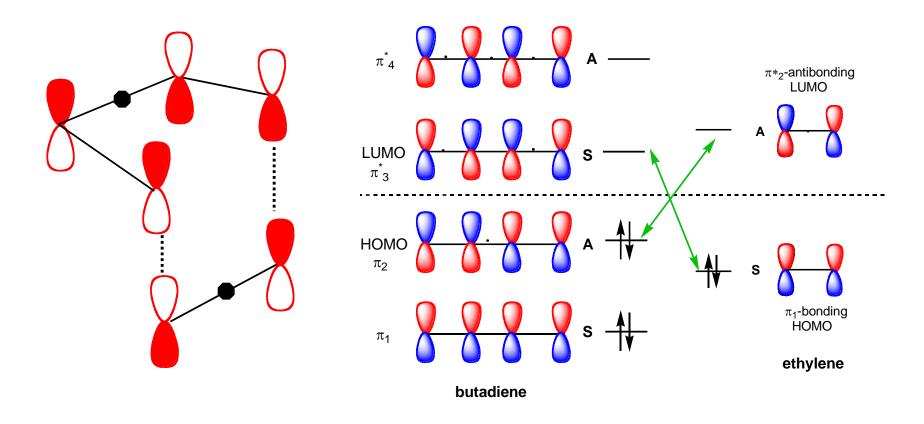


#### [4+2]-Cycloaddiitions of Propenyl System

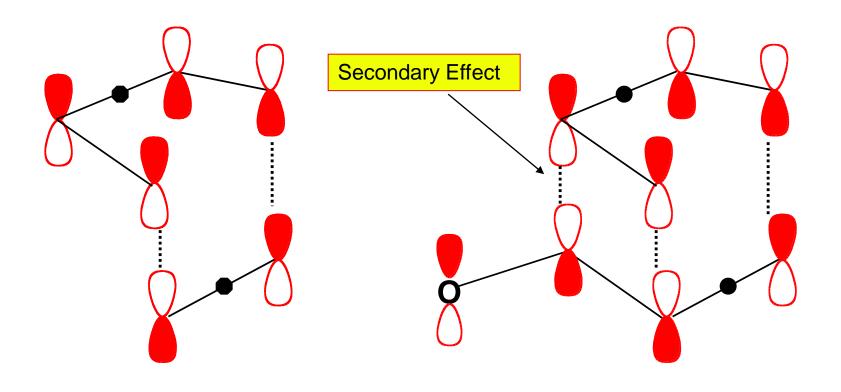




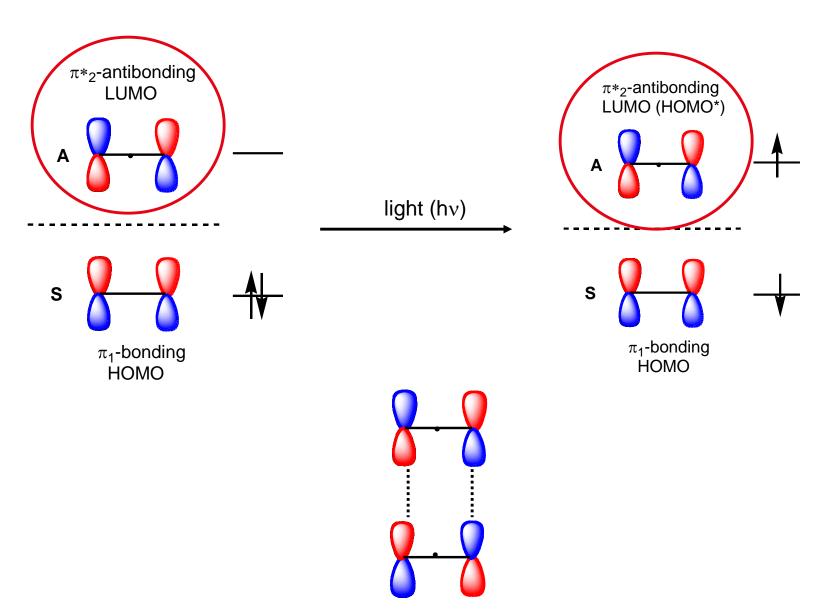
#### **Diels-Alder Reaction: Mechanism**



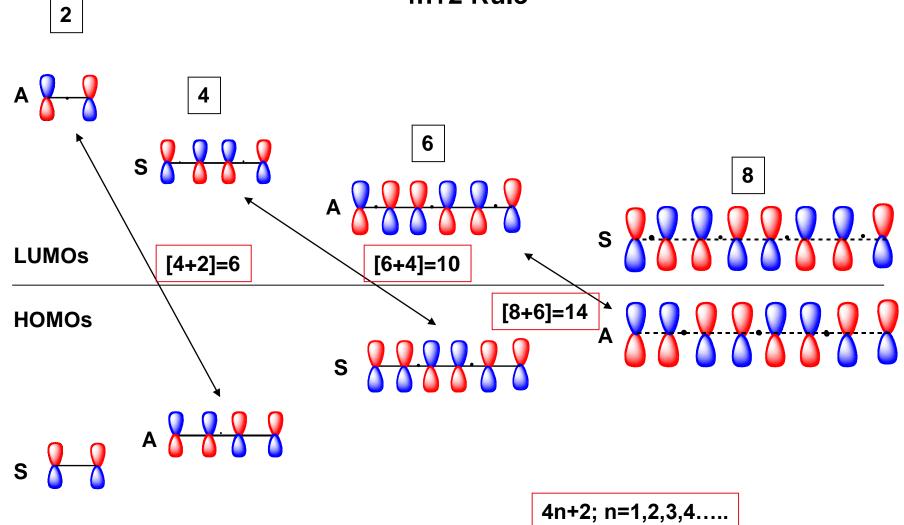
#### **Diels-Alder Reaction: The Endo Effect**



#### A [2+2] Cycloaddition Reaction



### Thermally Allowed Cycloadditions : Selection Rule 4n+2 Rule

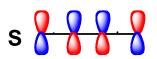


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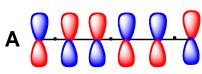
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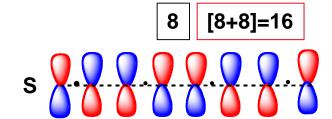
### Photochemically Allowed Cycloadditions :Selection Rule 4n Rule





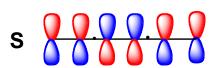


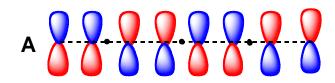


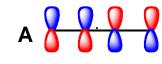


#### **LUMOs**

#### **HOMOs**







4n; n=1,2,3,4.....

and [2+6]=8; [8+4]=12

#### **Summary of Selection Rules of Cycloadditions**

		2	4	6	8	10
Thermal 4n+2	2	Р	Т	Р	Т	Р
	4	Т	Р	Т	Р	Т
Photochemical 4r	6	Р	Т	Р	Т	Р
	<b>8</b>	Т	Р	Т	Р	Т
	10	Р	T	Р	Т	Р

### Thank You



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