1st semester Organic Chemistry… Now in < 1 % the time!

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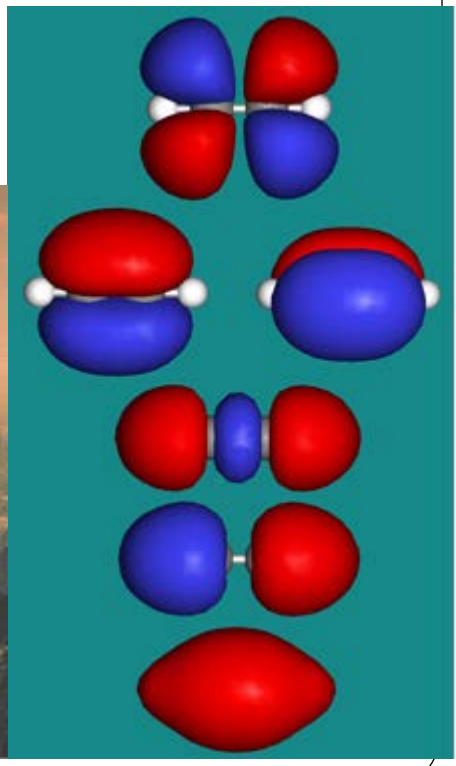
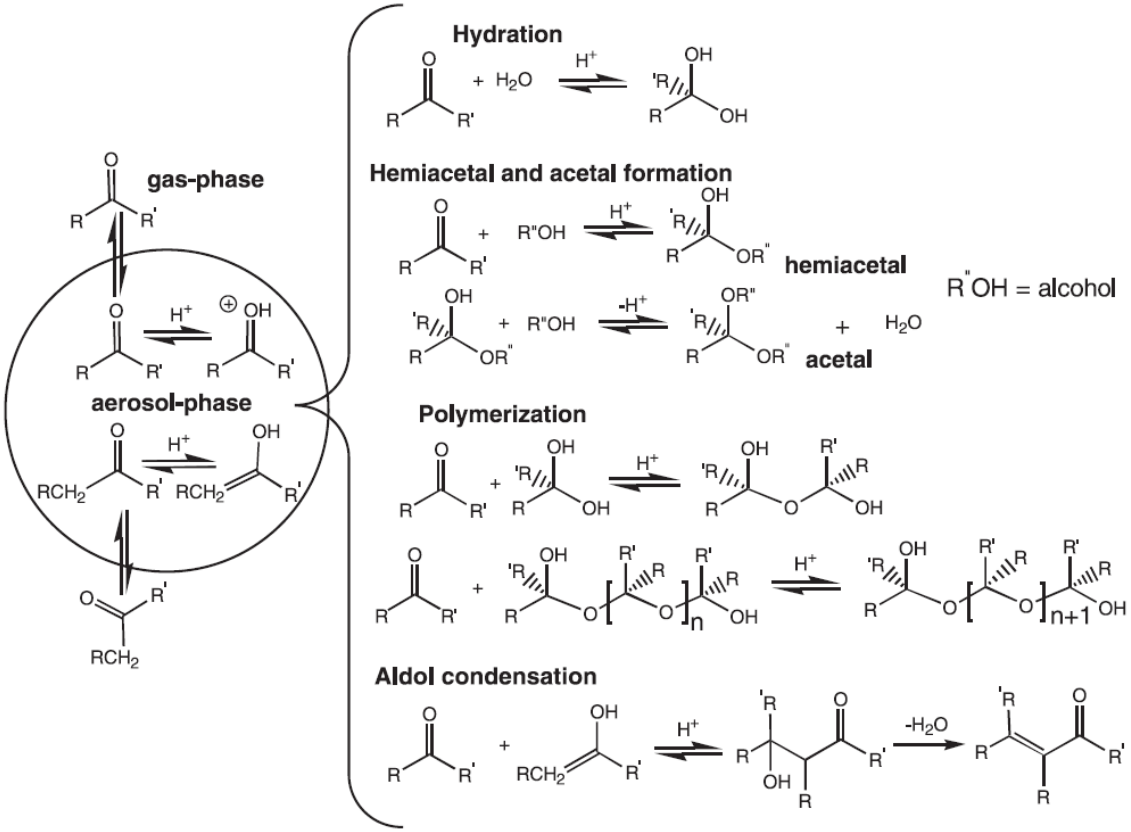
Jacob Group, Harvard EPS
Graduate Student Forum
January 12, 2012



What is going on?

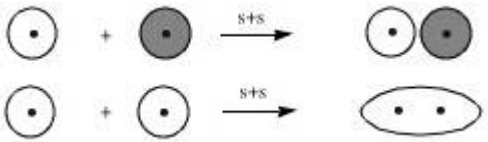
- Will a molecule react?
- What type of molecule will it react with?
- What bonds are likely to be created/destroyed?
- What will the product look like?



Molecular Orbitals

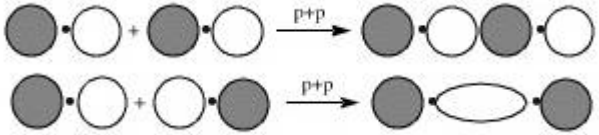
- 2 atomic orbitals combine constructively and destructively to form 2 molecular orbitals

Sigma orbital:
One region of overlap
corresponds to single bond



σ* antibonding

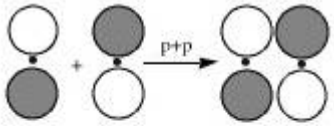
σ bonding



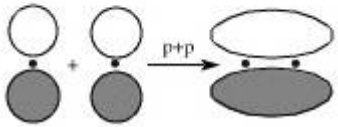
σ* antibonding

σ bonding

Pi orbital:
Two regions of overlap
corresponds to double bond



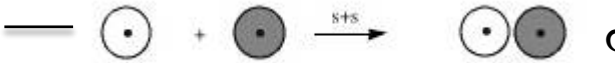
π* antibonding



π bonding

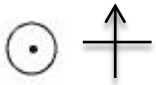
Molecular Orbital Example – H_2 vs. He

H_2 Molecule

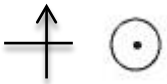


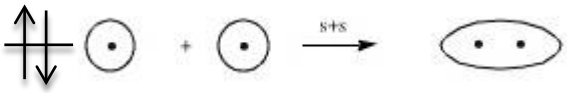
σ* antibonding

H Atom



H Atom

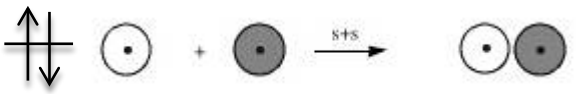




σ bonding

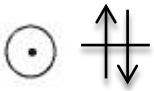
Molecular Orbital Example – H_2 vs. He

He_2 Molecule??

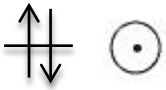


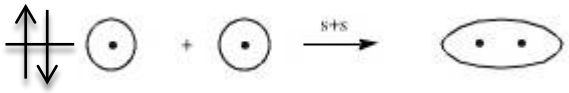
σ* antibonding

He Atom



He Atom

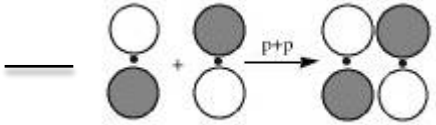




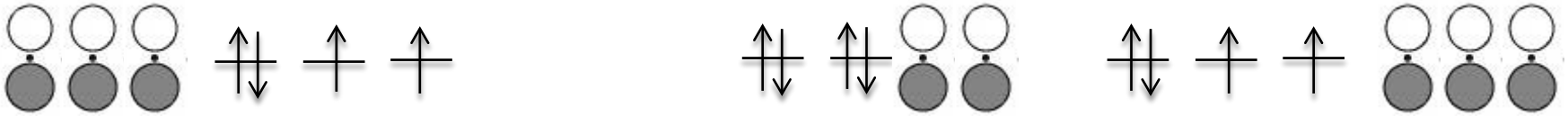
σ bonding

Molecular Orbitals – Relative Energy

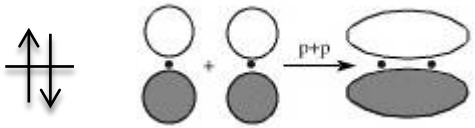
σ* antibonding



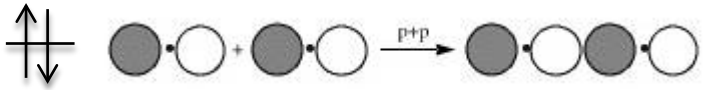
π* antibonding



(lone pairs)



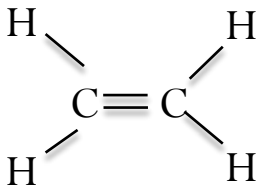
π bonding



σ bonding

Molecular Orbital Example -- Ethene

Ethene:



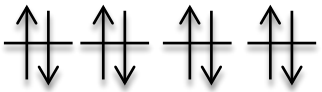
also written as:

C-C σ* antibonding

C-H σ* antibonding

C-C π* antibonding

C-C π bonding



C-H σ bonding

C-C σ bonding

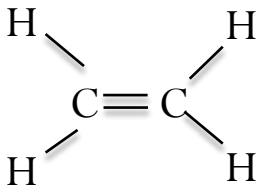
Frontier Orbitals – HOMOs and LUMOs

- Behaves as electron donor (i.e. Nucleophile, Lewis Base) at Highest Occupied Molecular Orbital (HOMO)
  - Lone pairs (or radicals)
  - π bonds

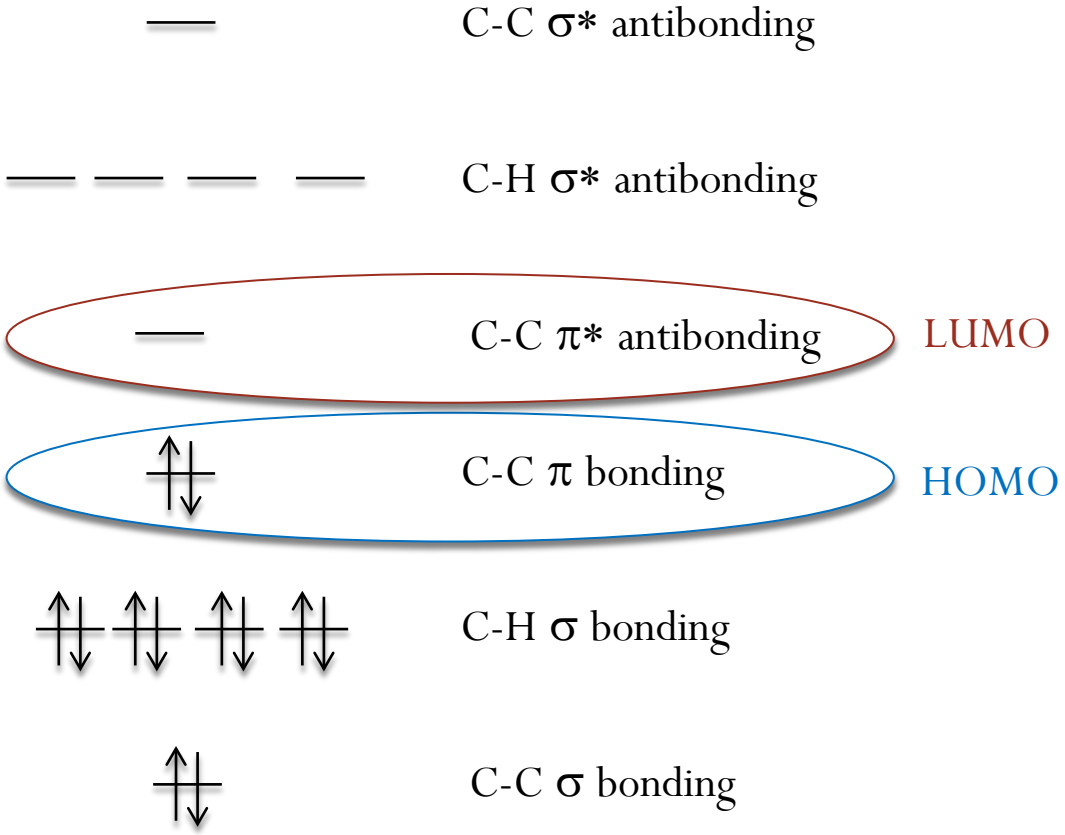
- Behaves as electron acceptor (Electrophile, Lewis Acid) at Lowest Unoccupied Molecular Orbital (LUMO)
  - Empty atomic orb.
  - π* antibonding orb.
  - σ* antibonding orb.

Molecular Orbital Example -- Ethene

Ethene:

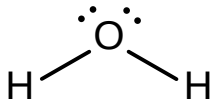


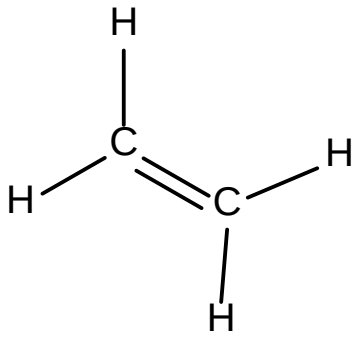
also written as:



Ethene Hydration

- What is the HOMO?

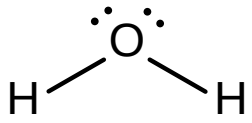


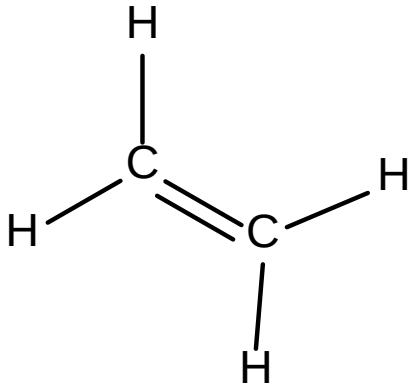


- What is the LUMO?

Ethene Hydration

- What is the HOMO?
  - O_2 lone pair





- What is the LUMO?
  - C-C π* antibonding orbital

Ethene Hydration

- What is the HOMO?
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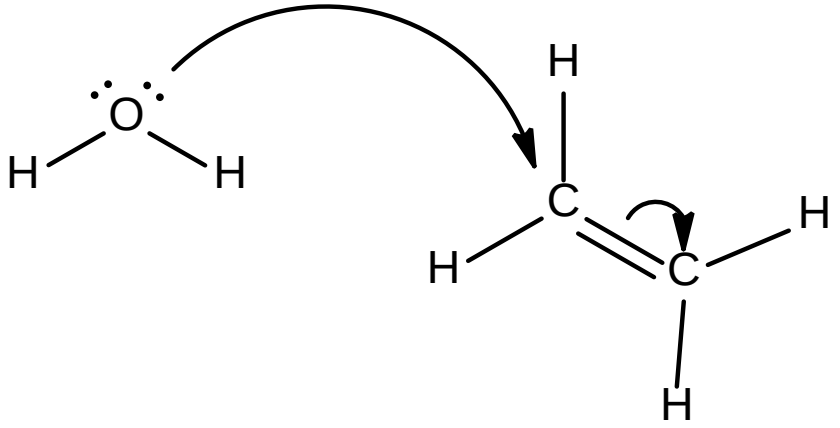

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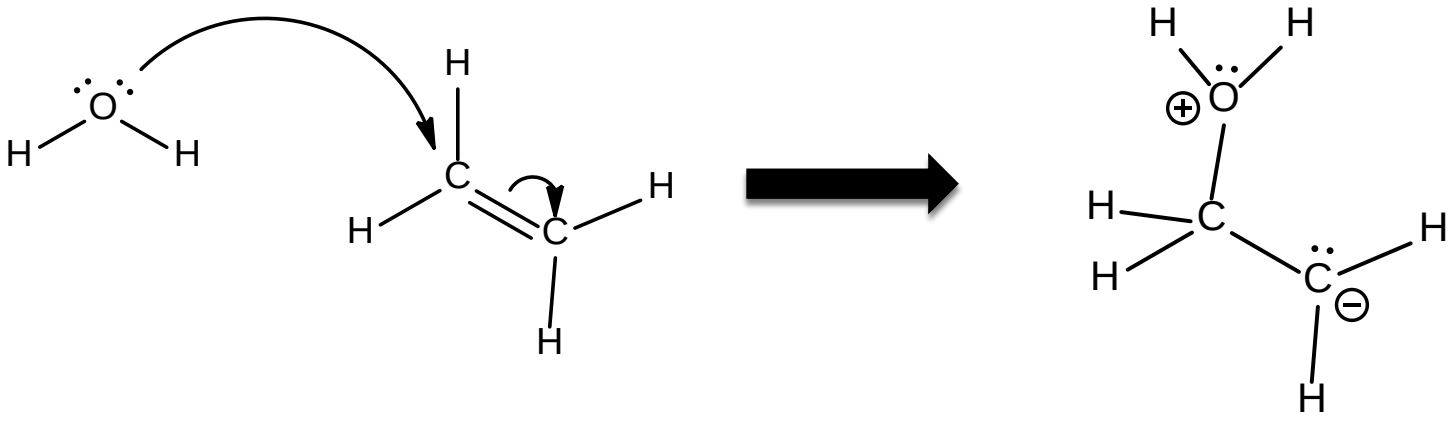
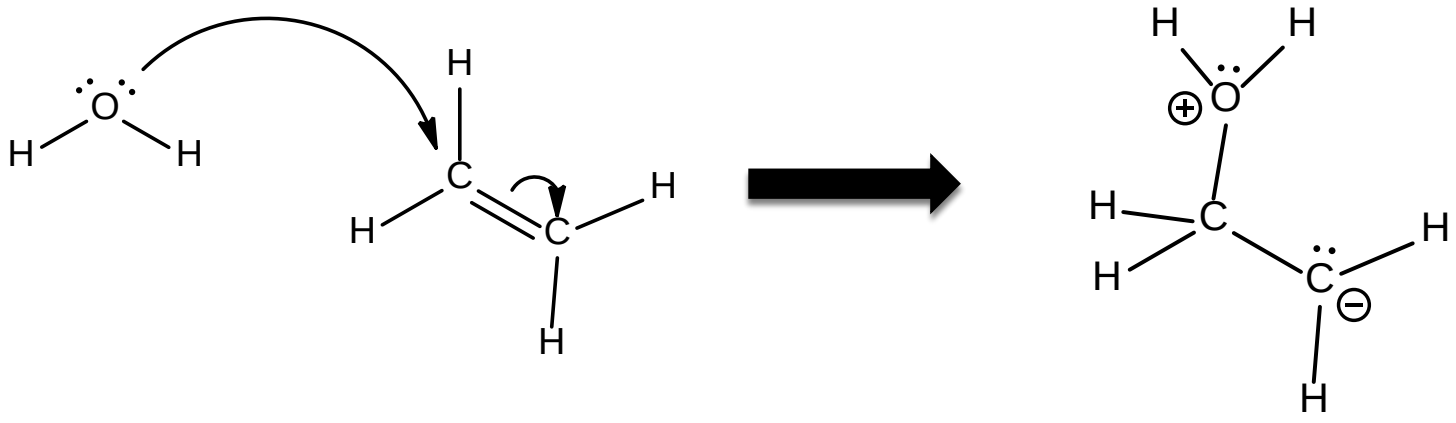
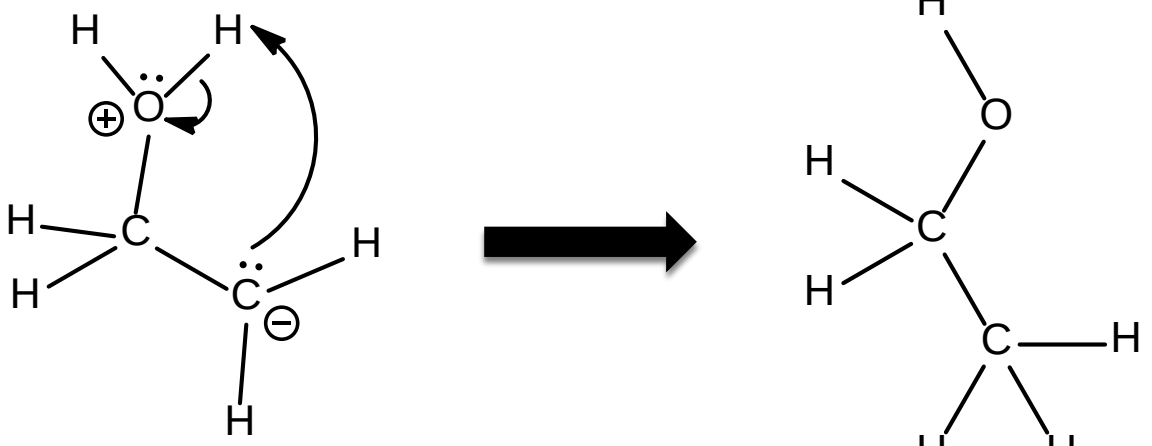
Ethene Hydration

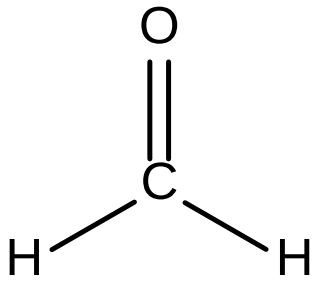


Ethene Hydration





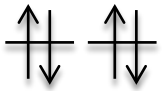
Molecular Orbitals -- Formaldehyde



C-H σ* antibonding

C-O σ* antibonding

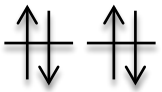
C-O π* antibonding



O Lone Pairs

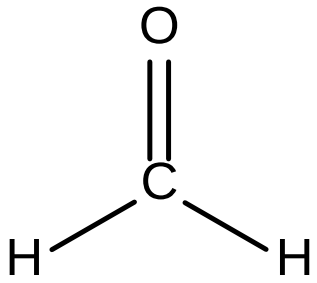
C-O π bonding

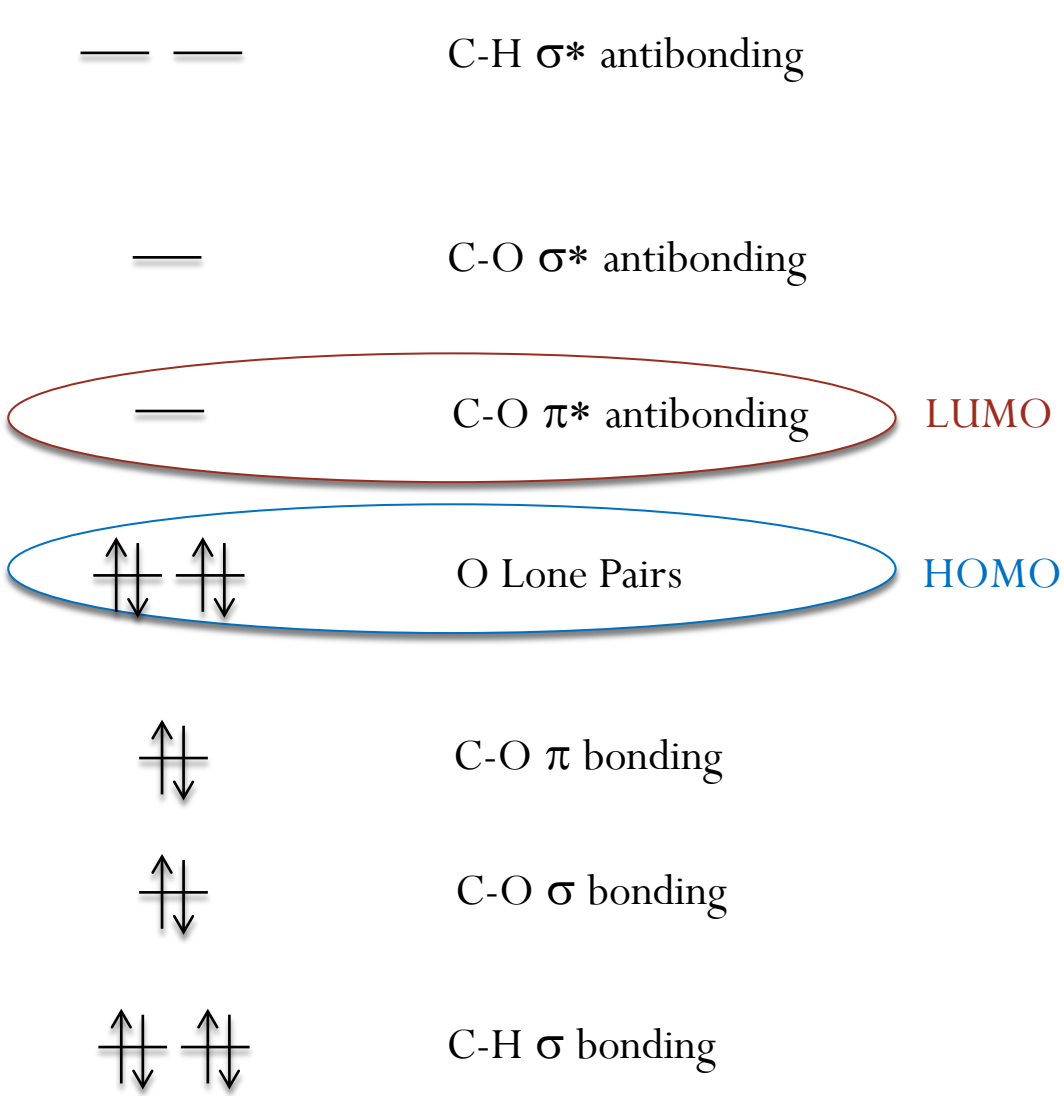
C-O σ bonding



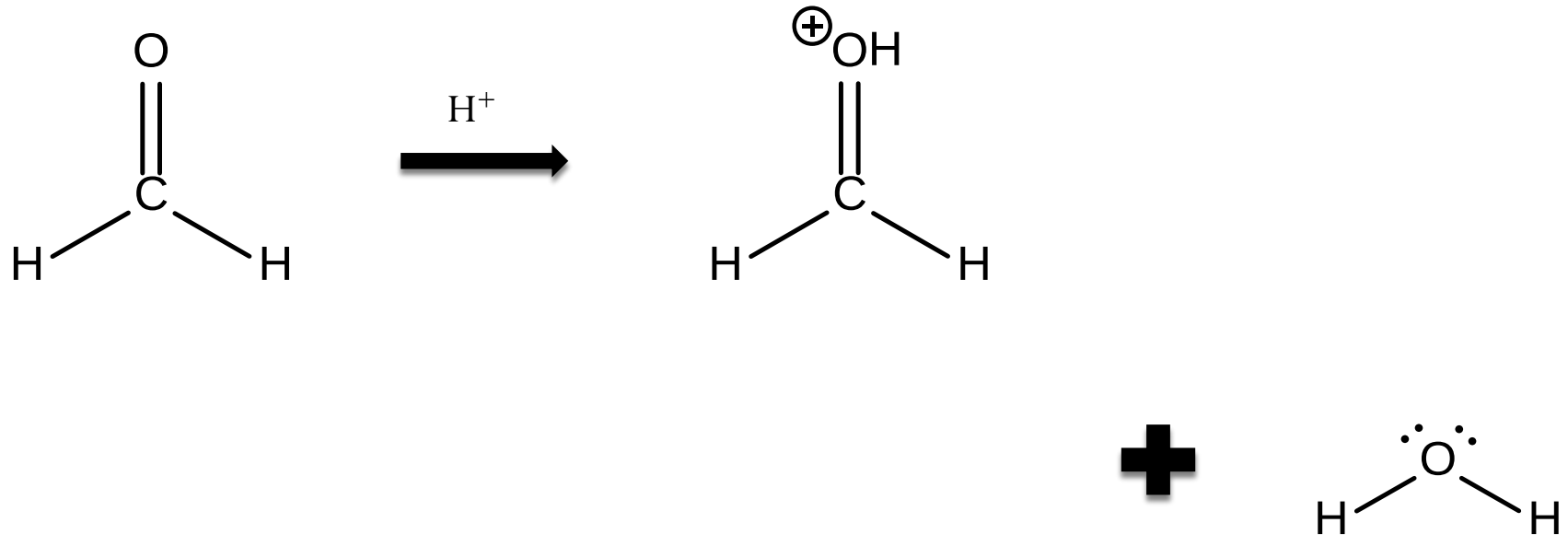
C-H σ bonding

Molecular Orbitals -- Formaldehyde





SOA formation by Polymerization



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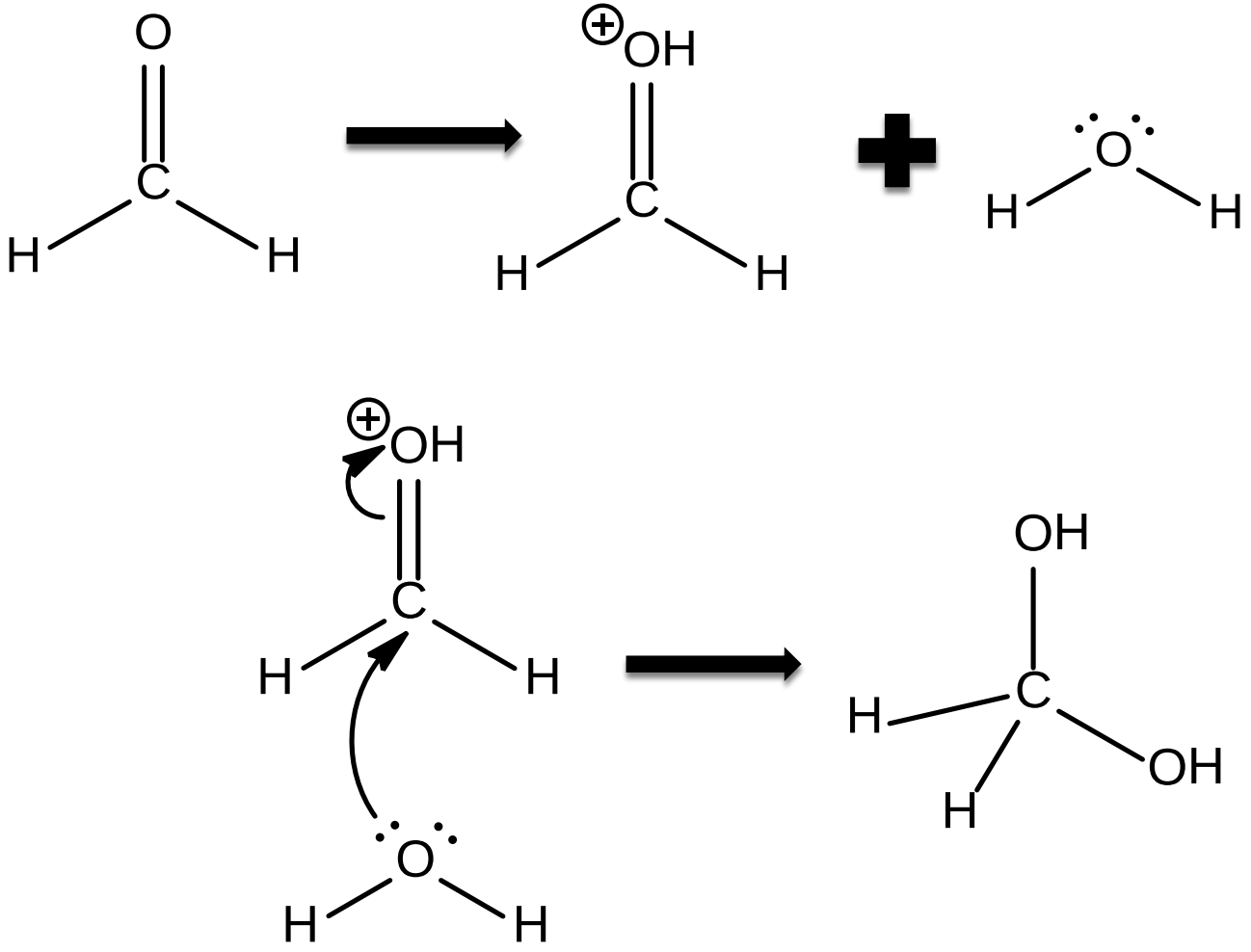

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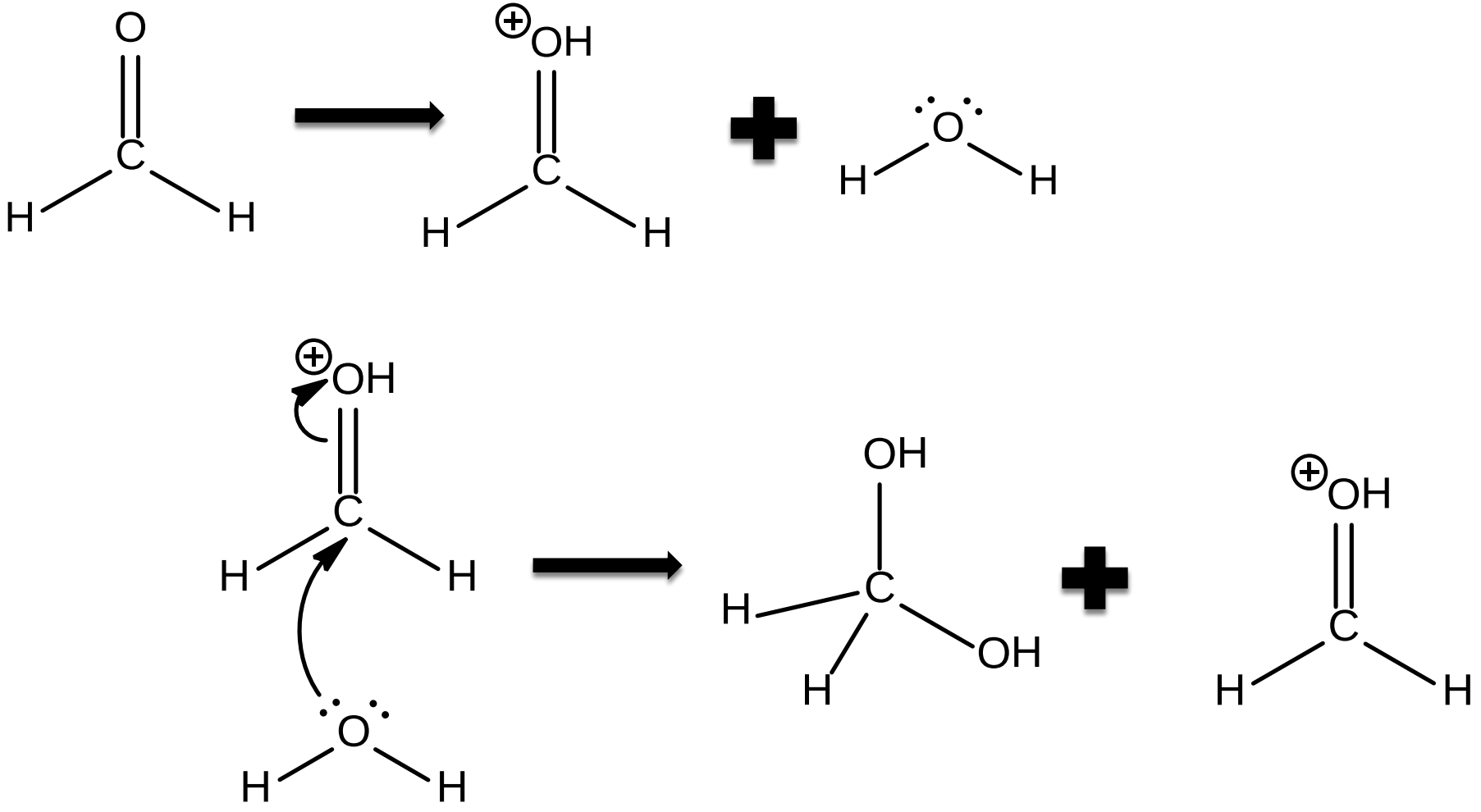
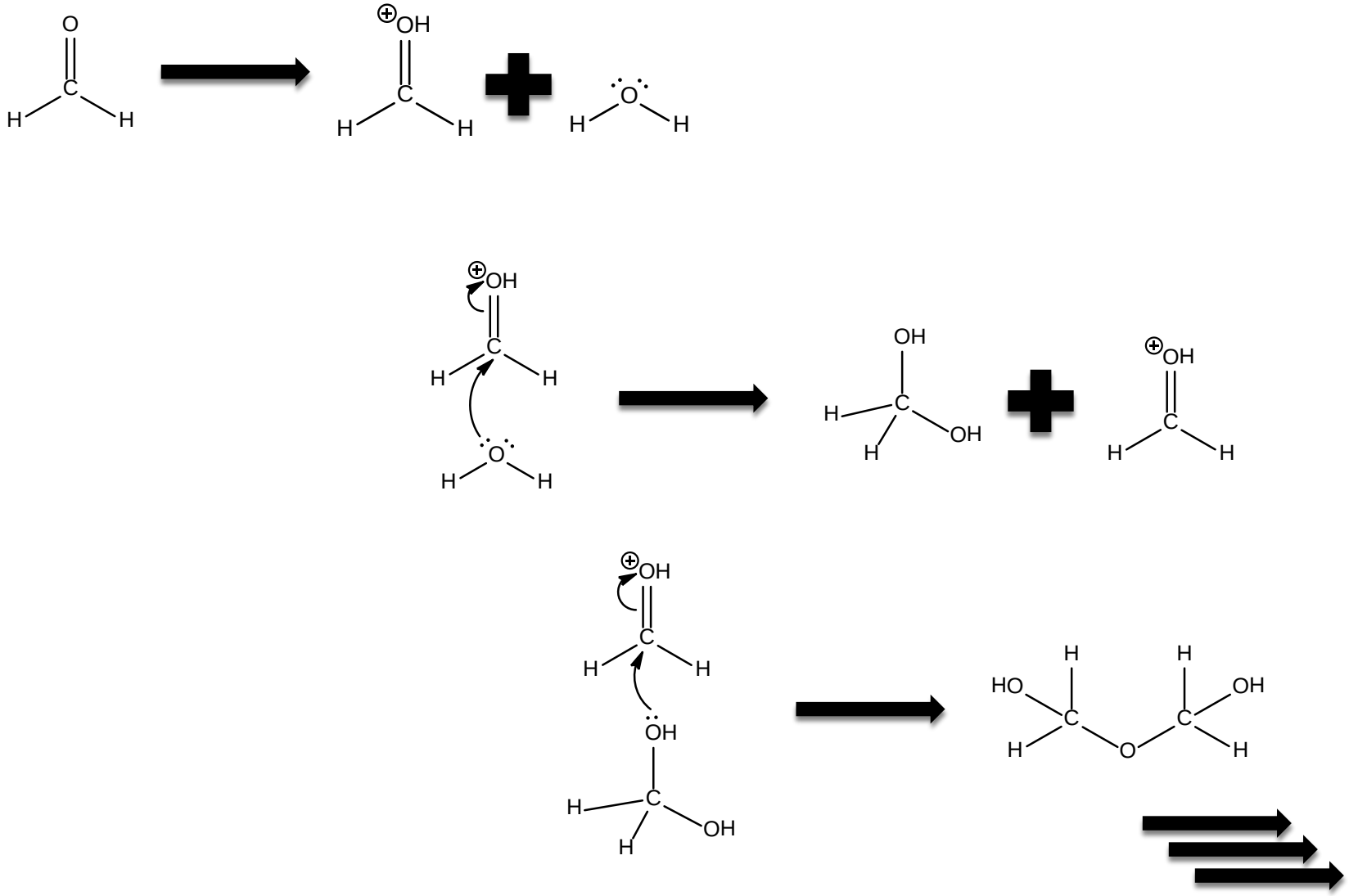


SOA formation by Polymerization



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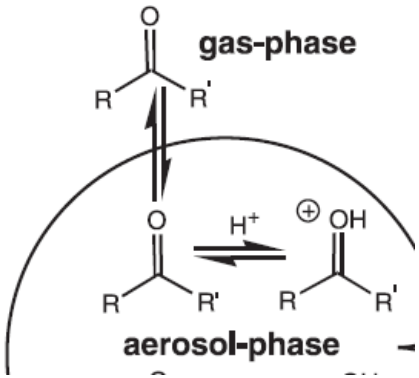

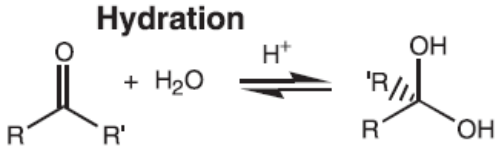

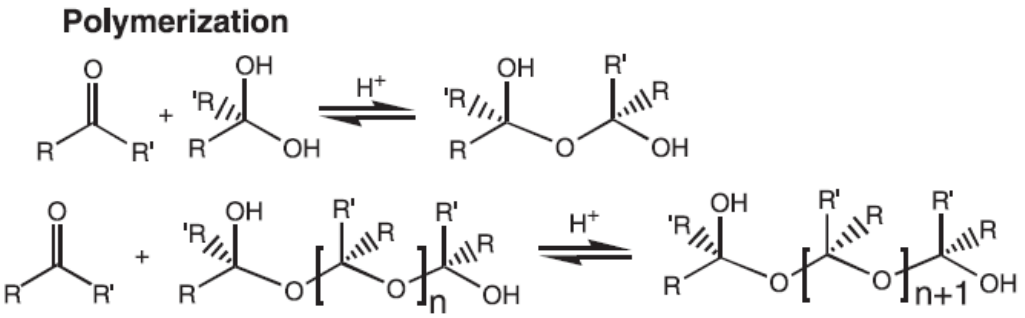

SOA formation by Polymerization