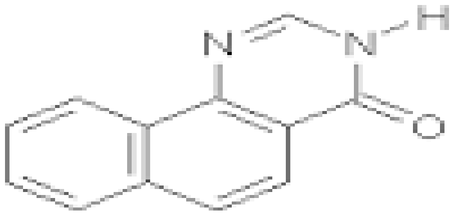
Organic pharmaceutical chemistry

Organic chemistry: Organic chemistry is the scientific study of the structure, properties, composition, reactions, and synthesis of organic compounds (molecules composed of carbon, hydrogen, and may contain any number of other elements like nitrogen,

oxygen and halogens).



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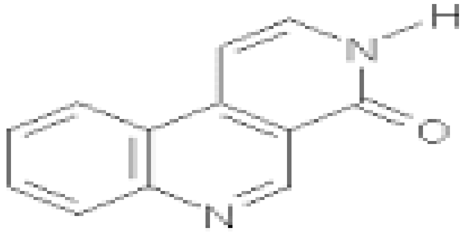

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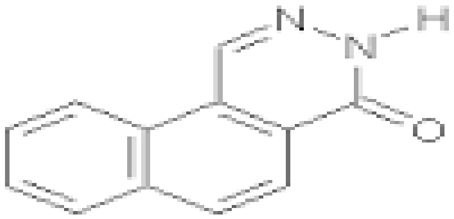

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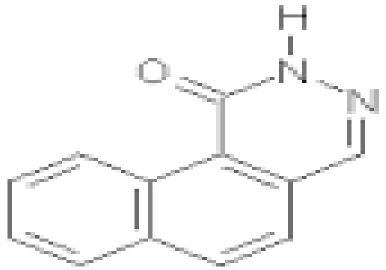

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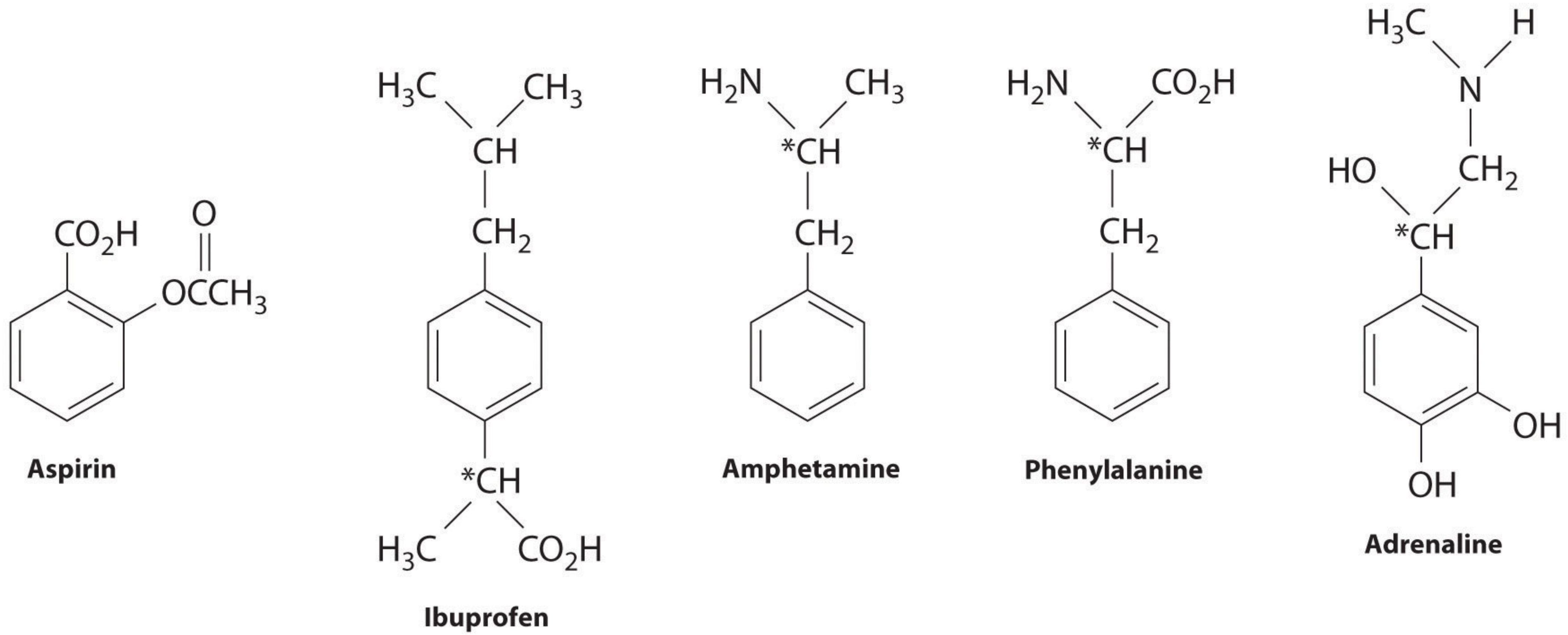
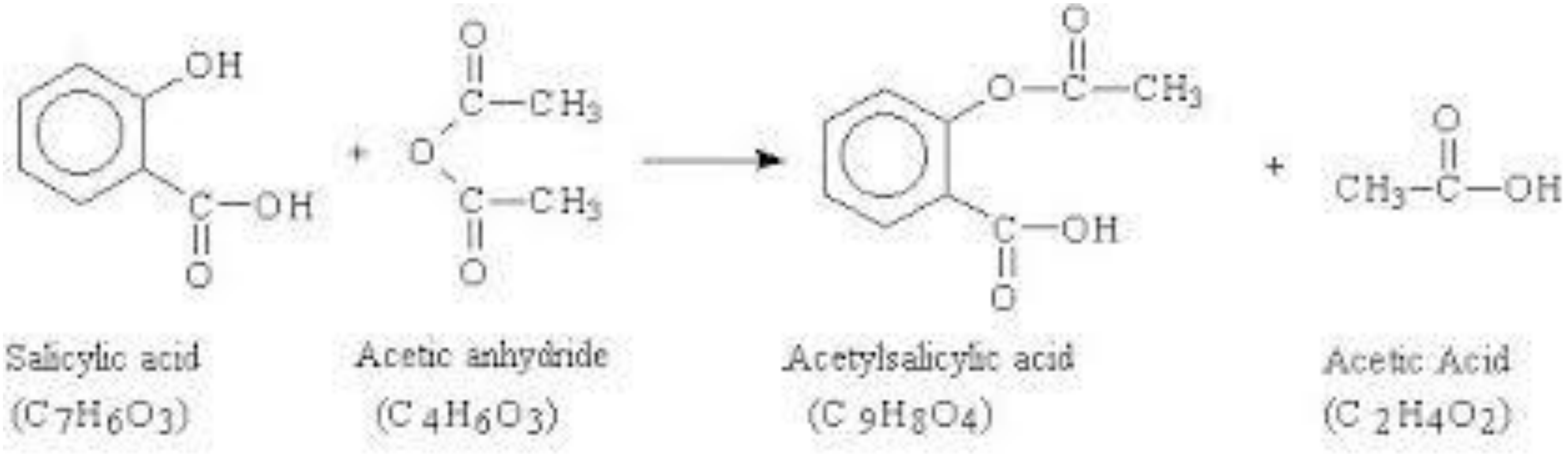
Organic pharmaceutical chemistry is the study of drugs, and it involves drug development. This includes drug discovery, delivery, absorption, metabolism, and more.



Aim of this lab: **synthesis of known drugs like aspirin, phenytoin, paracetamol…etc, through a suitable reactions depending on drug's molecular structure and the available chemicals and tools.**



Chemical reactions

Most molecules are at peace with themselves. Bottles of sulfuric acid, sodium hydroxide, water, or acetone can be safely stored in a laboratory cupboard for years without any change in the chemical composition of the molecules inside.

Reactions happen when electrons flow between molecules

- **When pair of molecules find themselves close together, a reaction can take place provided electrons move from one molecule to another. This is what we call the *mechanism of the reaction* (the detailed description of the pathway the electrons take).**
- **The molecule that accepts the electrons is called the *electrophile* (electron-lover).**
- **The molecule that donates the electrons is called the *nucleophile*.**

- A bond forms when electrons move from a nucleophile to an electrophile:

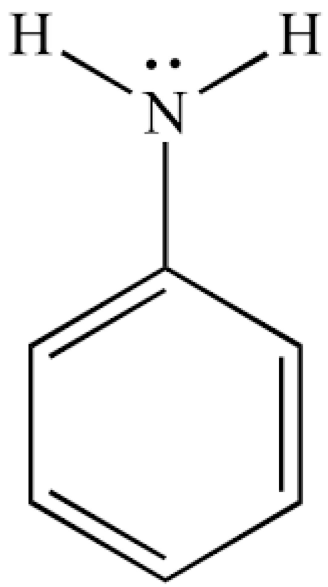
from nucleophile (Nu or Nu^-) — electron movement → to electrophile (E or E^+)

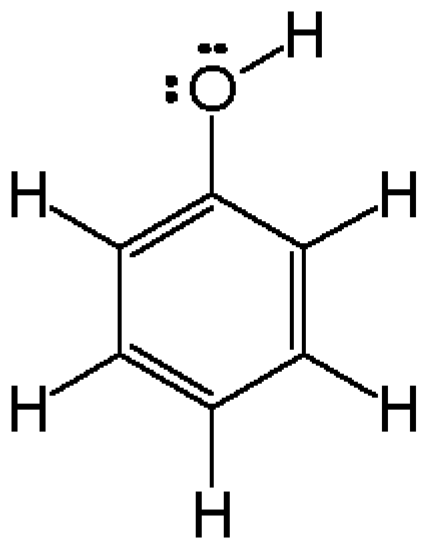
The nucleophile donates electrons.

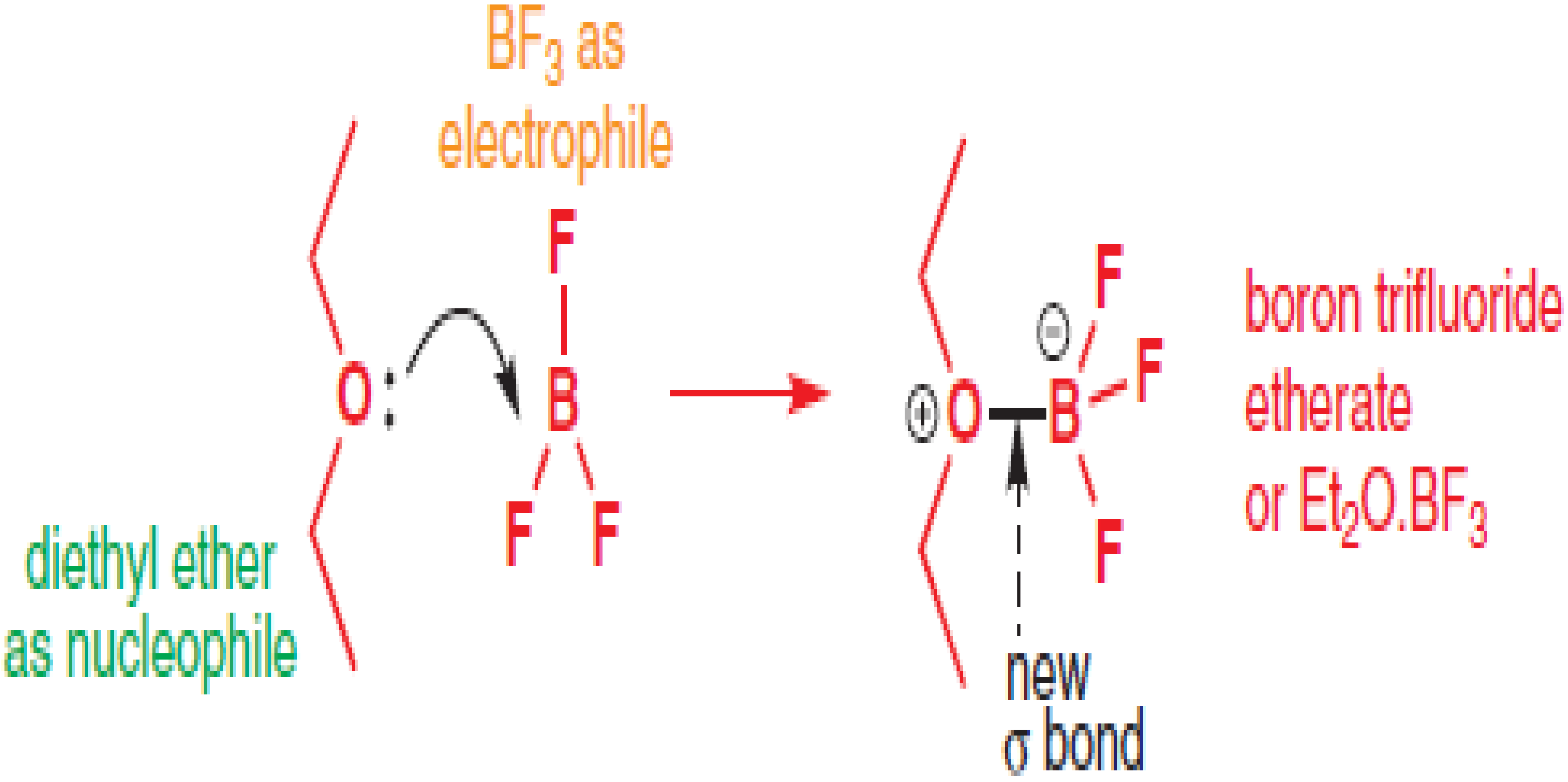
The electrophile accepts electrons.

Identifying a nucleophile

- **Neutral nucleophiles with lone pairs of electrons, typically: ammonia, amines, water, and alcohols, all of which have lone pairs (one for N, two of equal energy for O).**

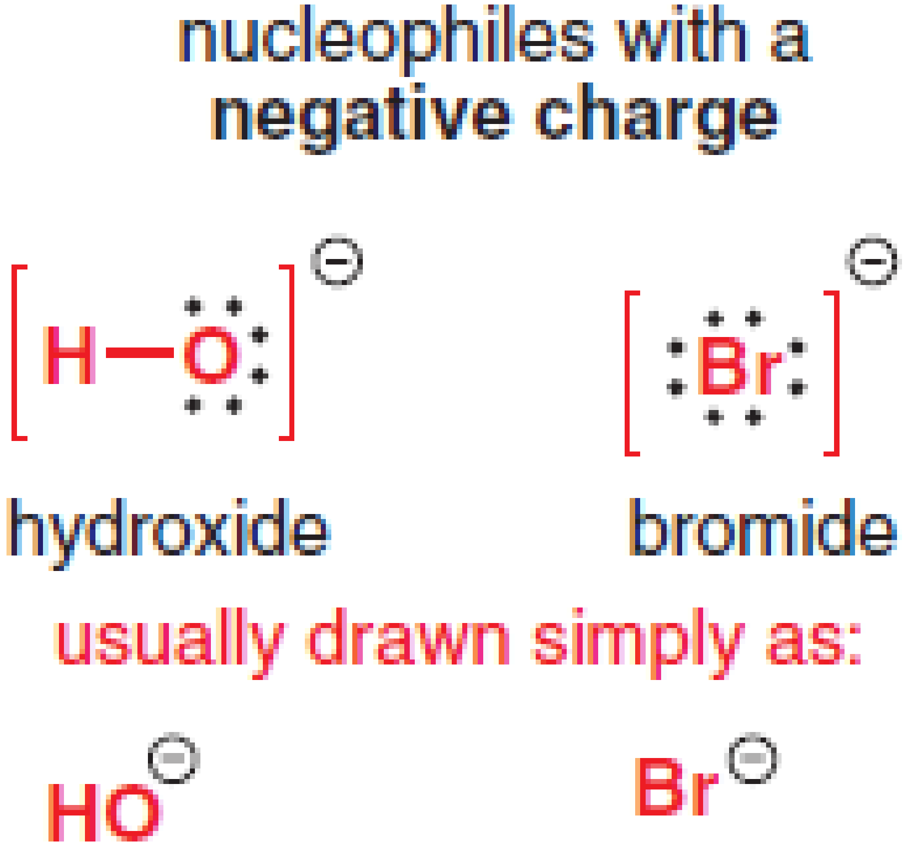


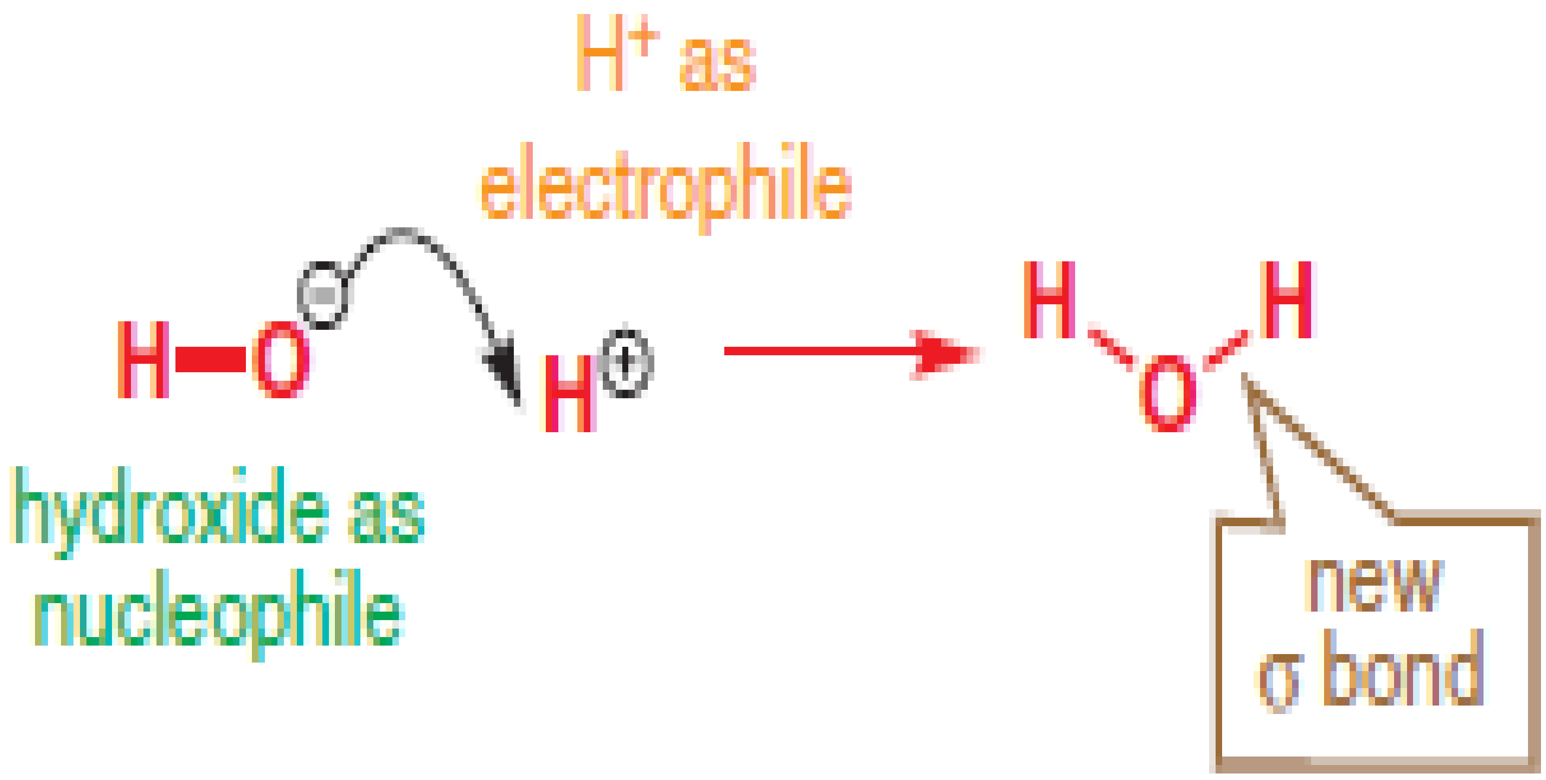




The arrow starts on the lone pair

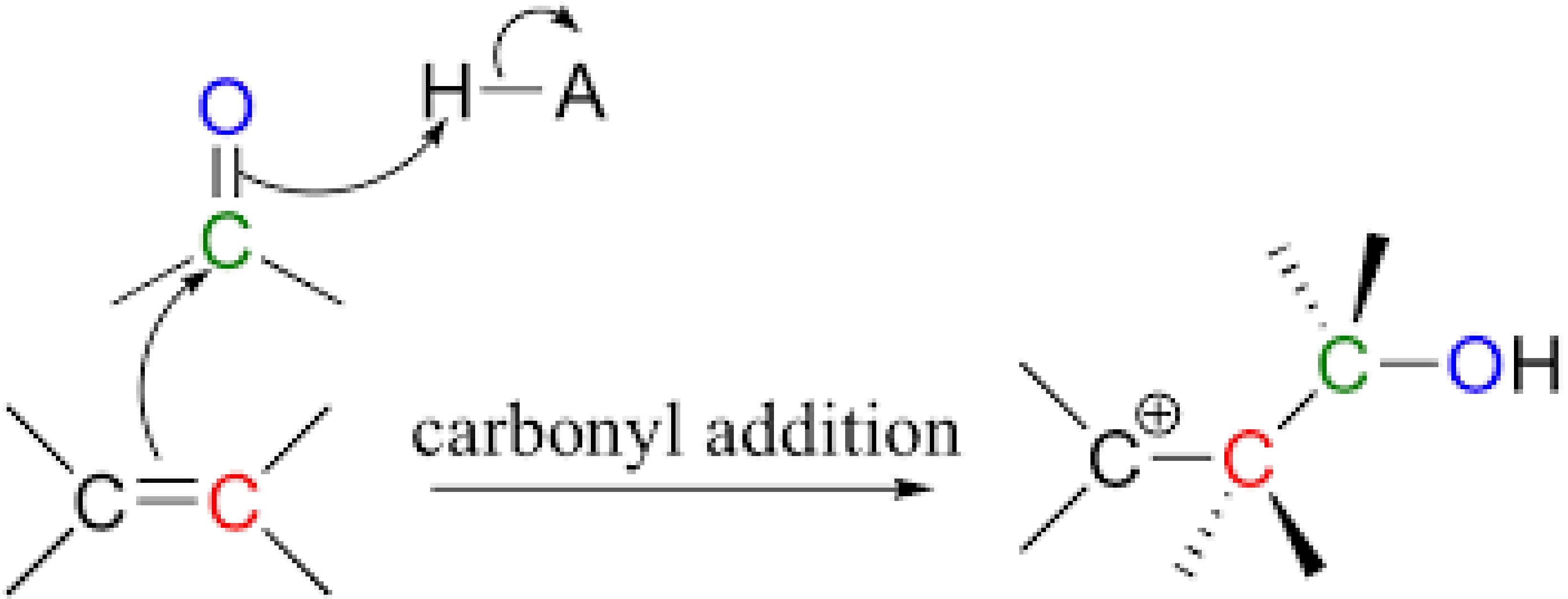
- **Negatively charged nucleophiles** are often good nucleophiles too, partly because they can be attracted electrostatically by positively charged electrophiles. The anionic centre is usually O, S, or halogen. For example, hydroxide.





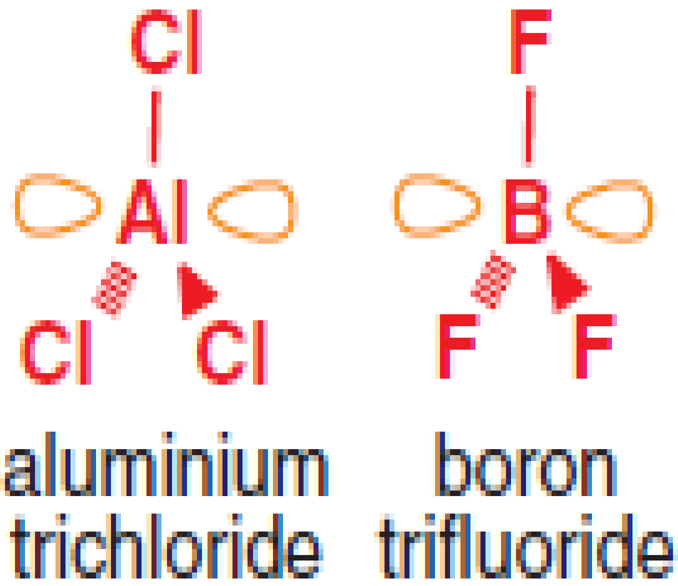
The arrow starts on the hydroxide's negative charge, which represents one of the oxygen's pairs of electrons

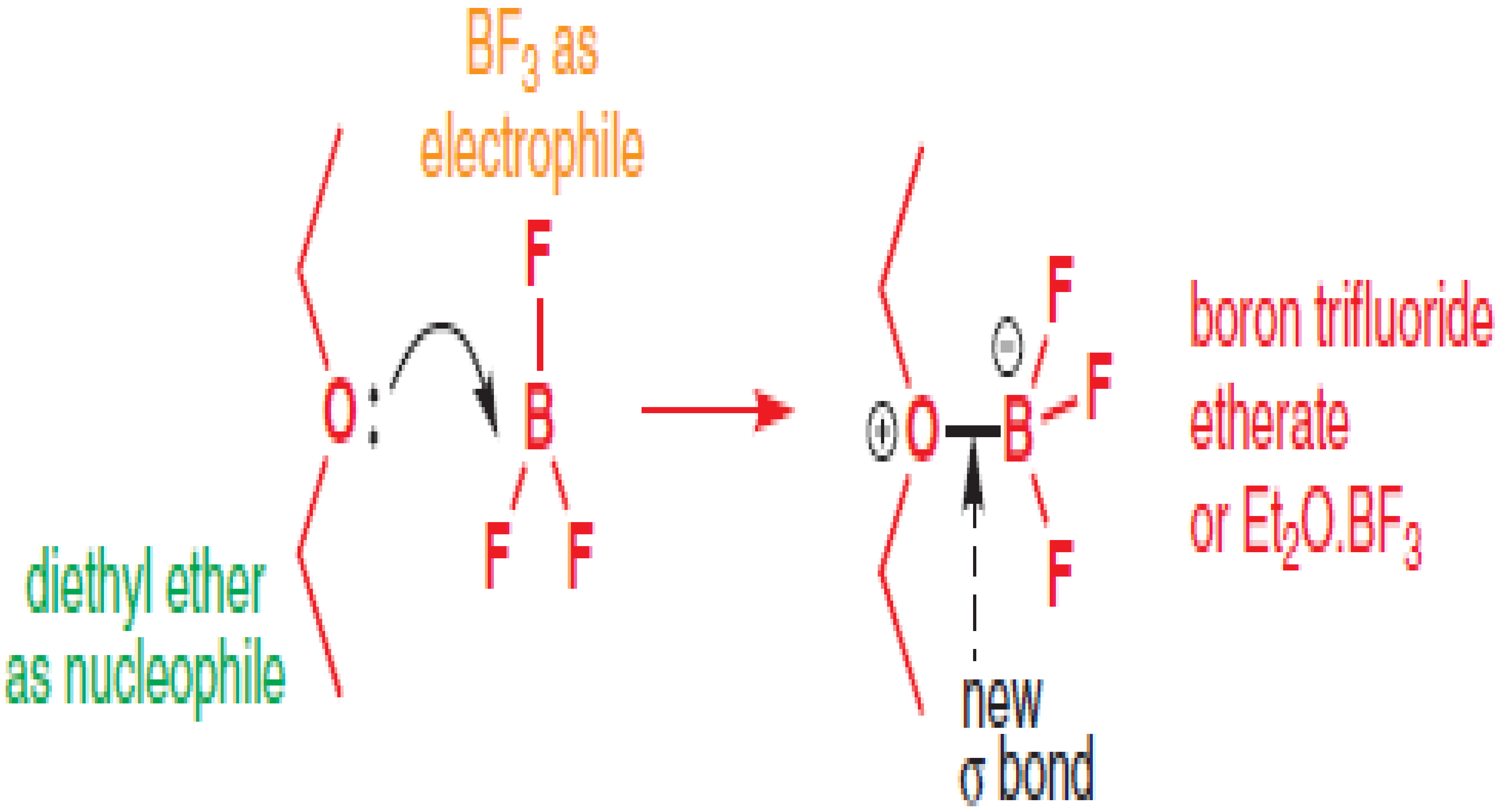
- **Bonding π orbitals**, especially **C=C** double bonds, since they are higher in energy than σ orbitals. The only common π nucleophiles are alkenes and aromatic rings.



Identifying an electrophile

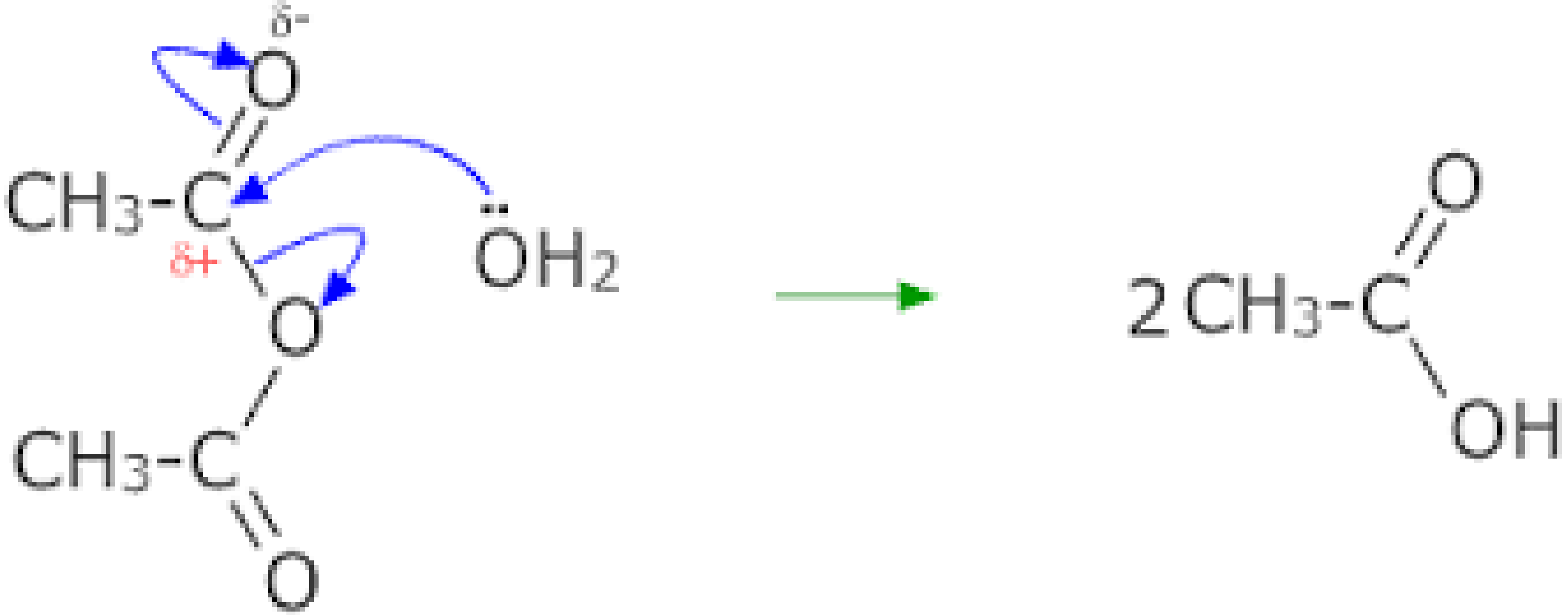
- **Neutral electrophiles with an empty atomic orbital that can easily accept electrons, such as boron trifluoride and aluminium trichloride.**



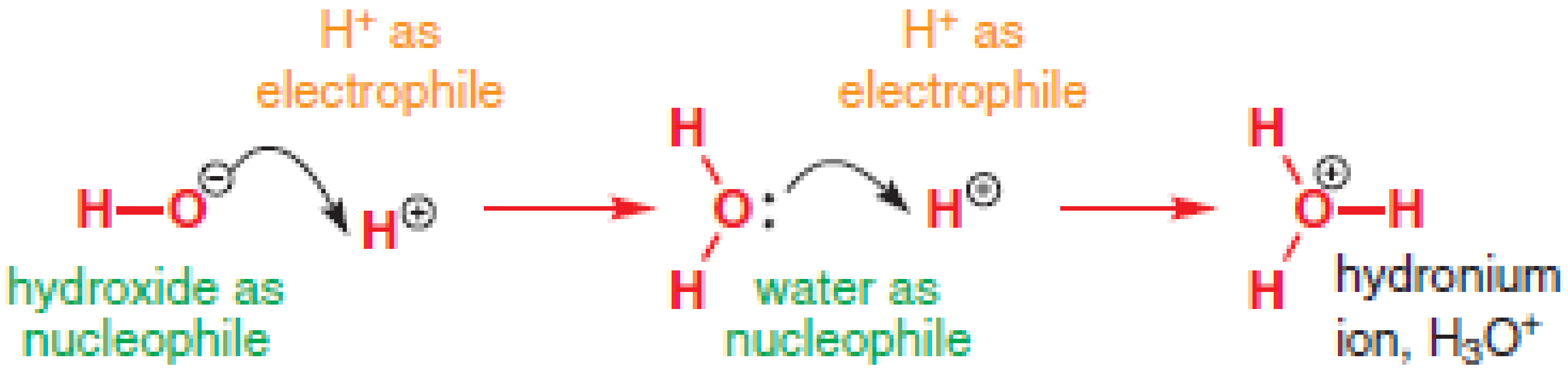

BF3 as electrophile
diethyl ether as nucleophile
O
B
F
F
F
O
B
F
F
F
new σ bond
boron trifluoride etherate or Et2O.BF3

- **Positively charged electrophile** like

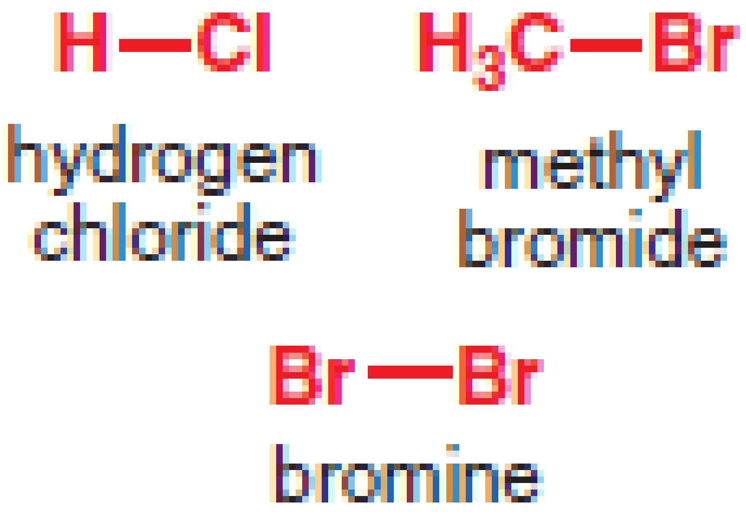
1. **Carbonyl group. There is a partial positive charge on the carbon and a partial negative charge on the oxygen, because oxygen is more electronegative than carbon. So the oxygen pulls electrons towards itself.**



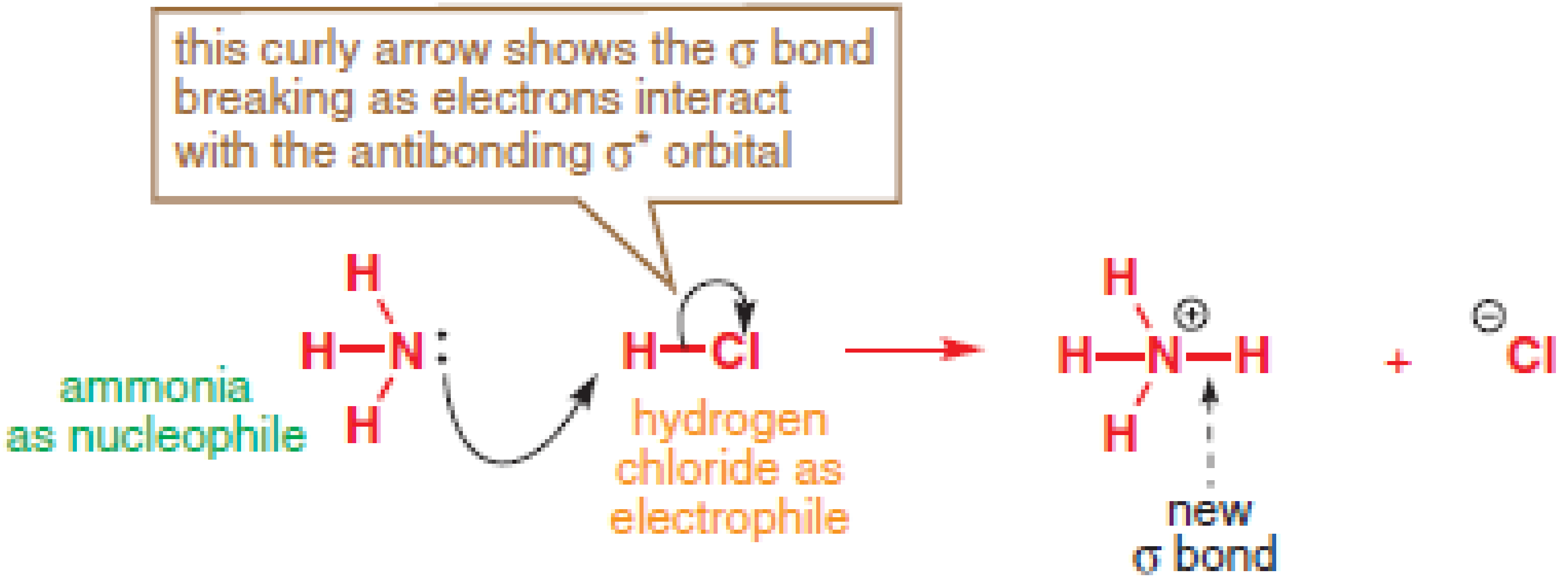
2 - The simplest electrophile is the hydrogen cation, H+, usually named for what it is, a proton. H+ is a species without any electrons at all. It is so reactive that it is hardly ever found and almost any nucleophile will react with it.



3. Molecules with a single bond to electronegative atoms can also make good electrophiles, such as HCl or CH3Br. The dipole attracts the electrons of the nucleophile to the H or C atom.



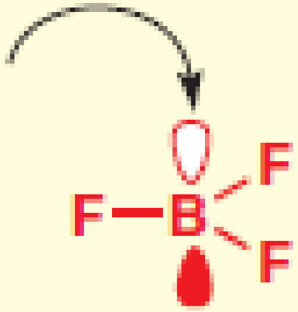
Example



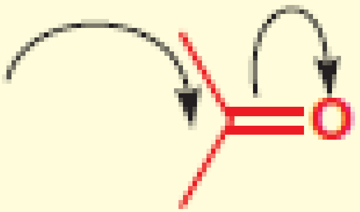
It is an **acid-base** reaction. All acid–base reactions are reactions between a nucleophile (the base) and an electrophile (the acid). We call an electrophile an acid if is has an **X–H** bond (**X** being any atom) that loses **H+** in its reactions. We call a nucleophile a base when it uses a **lone pair** to donate electrons to the **X–H** bond.

- **Electrophiles accept electrons into empty low-energy orbitals represented by one of the following:**

a positive charge representing an empty orbital



a neutral molecule with an empty p orbital



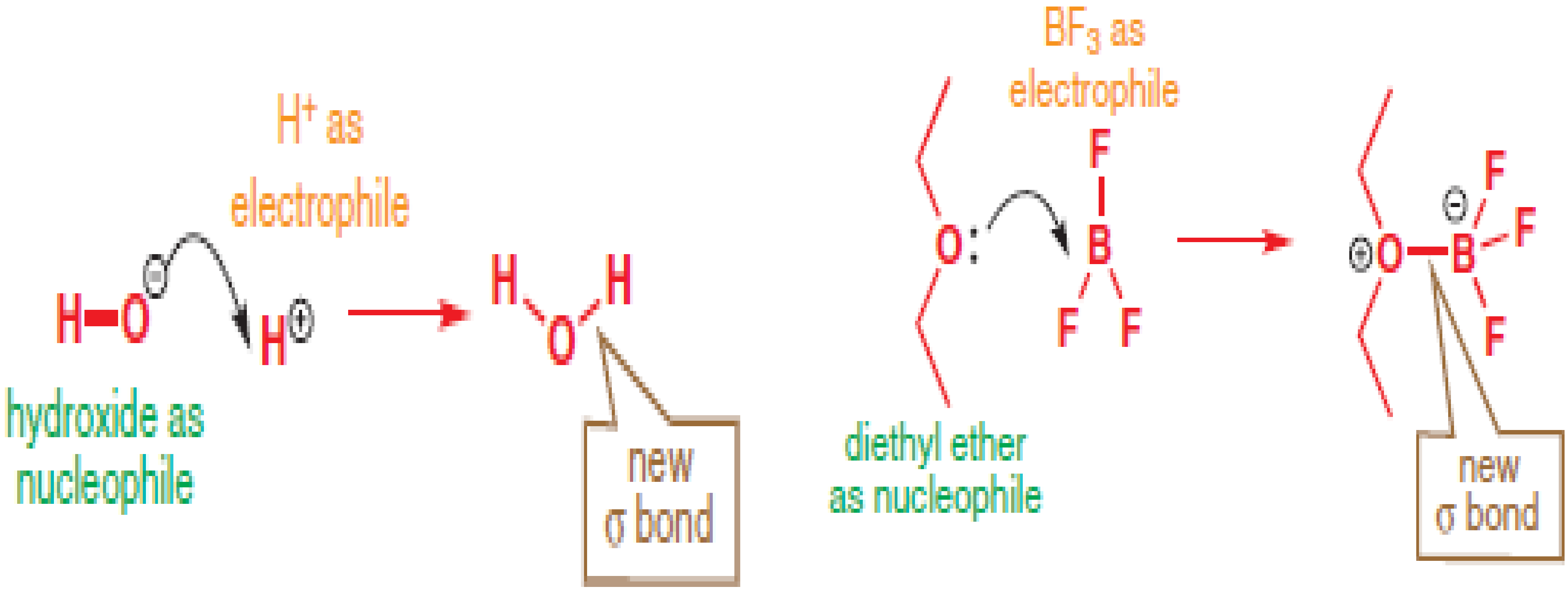
a double bond to an electronegative element

a single bond to an electronegative element

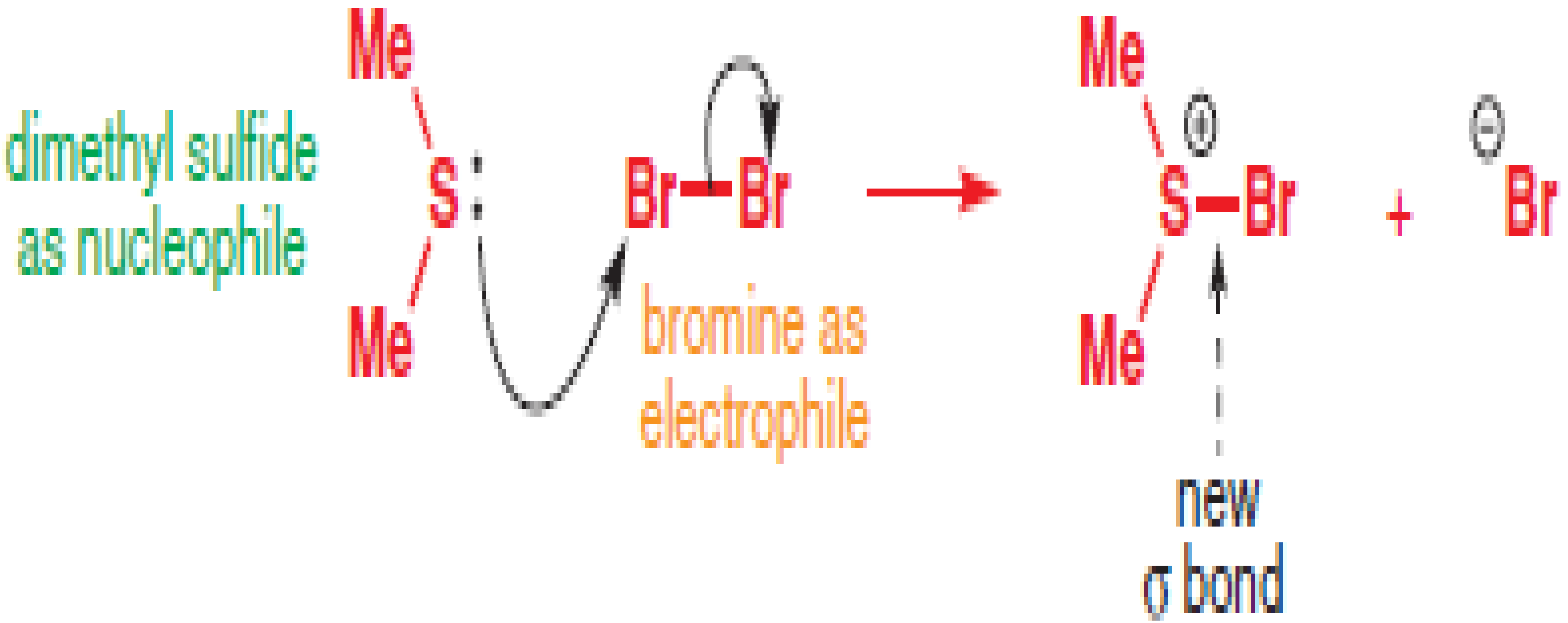
Curly arrow

A curly arrow represents the *movement of a pair of electrons* from a filled orbital into an empty orbital. The result of this movement is to form a bond between a nucleophile and an electrophile.

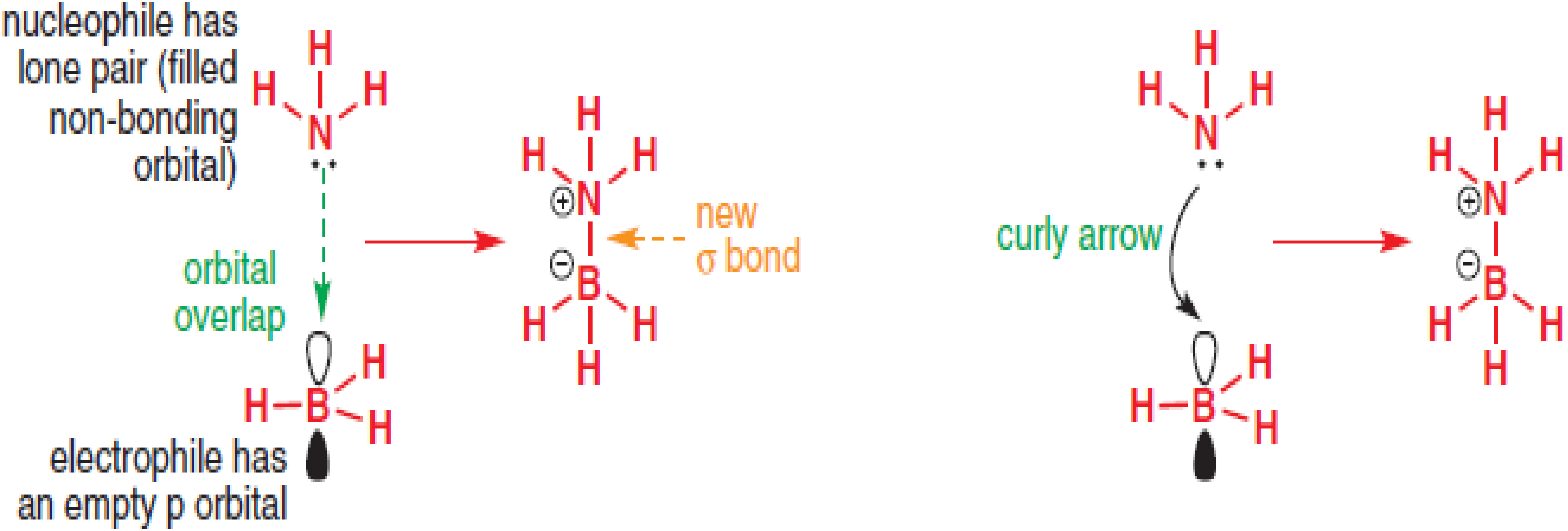
- Arrow to **make new bond**



- Arrow to **break** an **old bond**



Example

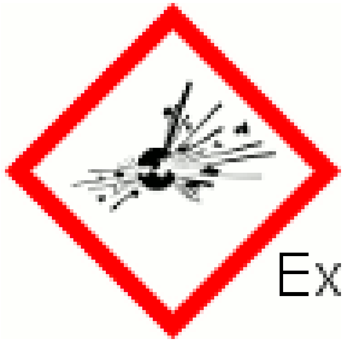


Electrons flow from the ***nucleophile*** ($NH3$) to the ***electrophile*** ($BH3$) and a new bond is formed.

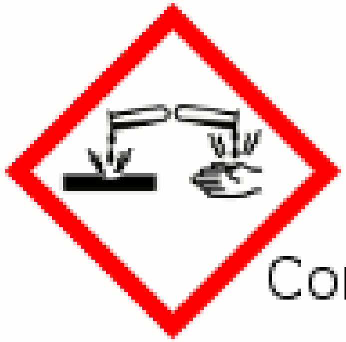
Chemistry Laboratory Safety Rules

1. **Always Follow the Instructions.**
2. **Do Not Pipette by Mouth - Ever.**
3. **Read the Chemical Safety Information**. A Material Safety Data Sheet (MSDS) should be available for every chemical you use in the lab.
4. **Don't Taste or Sniff Chemicals**
5. **Dress Appropriately** (include a lab coat, safety goggles and gloves).

Hazard symbols



Explosive

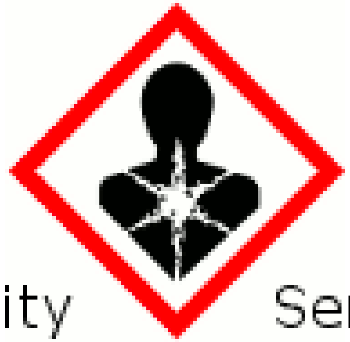


Corrosive

Health Hazard

Flammable

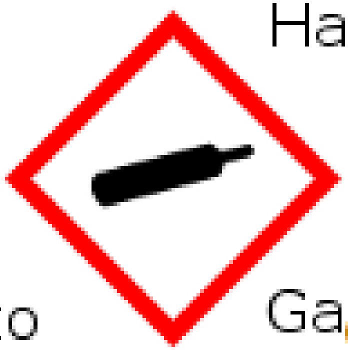
Acute Toxicity



Serious Health Hazard

Oxidising

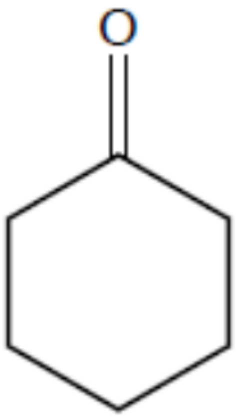
Hazardous to the environment

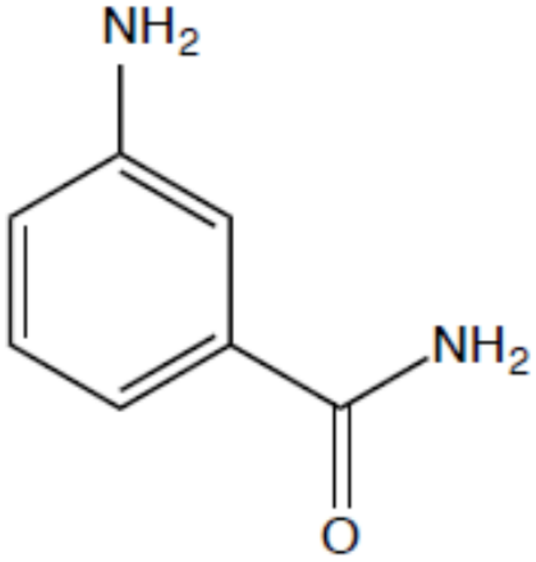


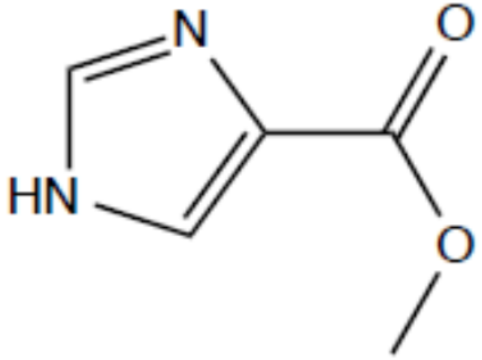
Gas Under Pressure

Home work

1- Draw the lone pairs on the following structures







2- Complete these mechanisms by drawing the structure of the products(s)