Chemistry

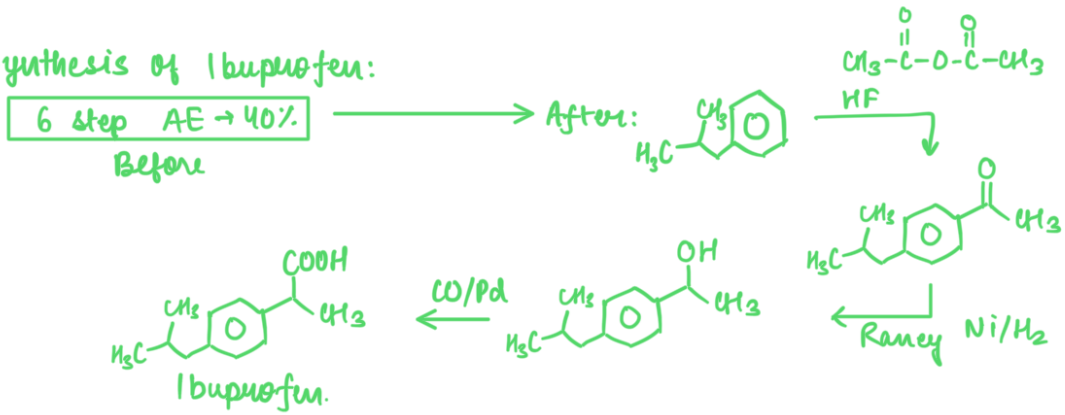
Green Chemistry:

12 principles of Green chemistry:
- Prevention
- Atom Economy
- Less Hazardous chemical Synthesis
- Design Safer chemicals
- Safer Solvents and Auxiliaries
- Design for Energy Efficiency.
- Use of Renewable feedstocks.
- Reduce Derivatives
- Catalysis
- Design of Degradation.
- Real time Analysis for Pollution Prevention.
- Inherently safer chemistry for Accident Prevention.

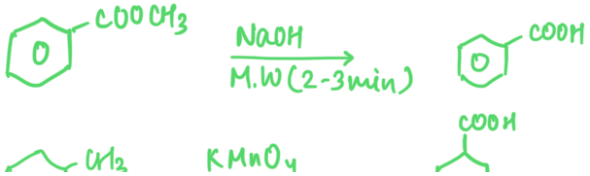
① **Prevention of waste:** It is better to prevent waste than to treat or clean up waste.
- cleaning & treatment add up to the cost.
- Carry out synthesis in which formation of waste is minimal.

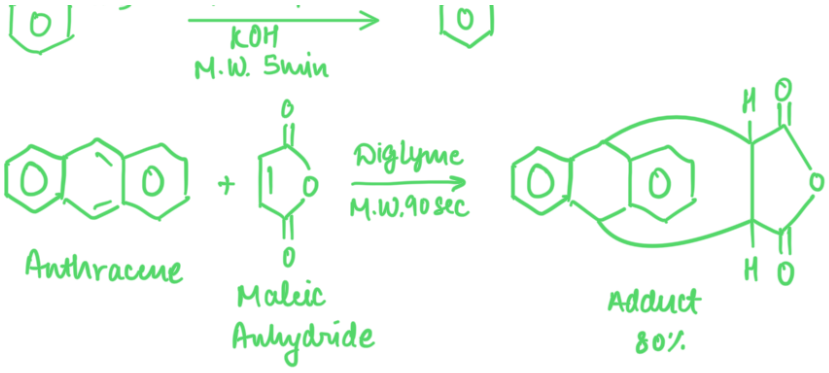
* Synthesis of Ibuprofen:

6 step AE → 40%
Before



* Microwave Induced Green Synthesis: 30GHz – 300Hz Home appliances → 2.45GHz





E-factor = $\frac{\text{mass of total waste}}{\text{Mass of desired product.}}$

② **Atom Economy:** Synthetic methods should be designed to maximize the incorporation of all materials (starting materials and reagents) used in the process into the final product.

* percentage yield = $\frac{\text{actual mass of product}}{\text{theoretical mass of product}} \times 100\%$

* Atom Economy = $\frac{\text{mass of atoms in desired product}}{\text{mass of atoms in reactants}} \times 100\%$

* Organic Rxns: 1) Addition Rxn → 100% Atom Economy
2) Elimination → not 100% Atom Economy
3) Substitution → not 100% Atom Economy
4) Rearrangement → 100% Atom Economy
5) Hofmann elimination → economy 35.30%
6) Dehydrohalogenation → economy 27%

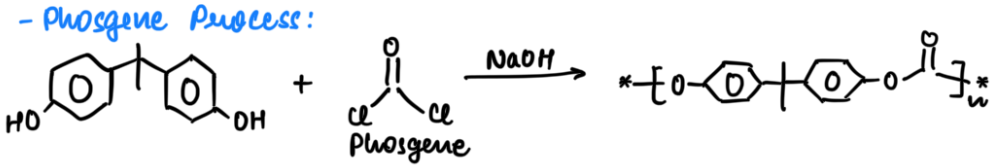
③ **Less Hazardous chemical synthesis:** Whenever practicable, synthetic methodologies should be designed to use and generate substances that possess little or no toxicity to the environment and the human health.

Risk = f {Hazard, Exposure} Eliminate the Hazard, no need to worry about the exposure.

* thalidomide was used for lessening the effects of nausea and vomiting during pregnancy. It causes defected child birth. Thus this drug was banned.

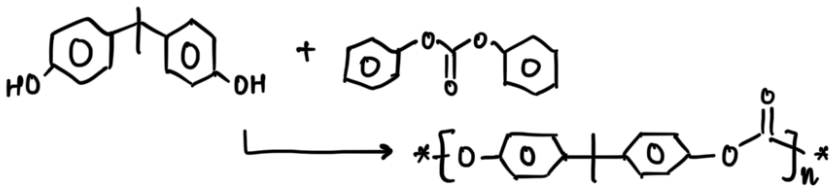
* Polycarbonate Synthesis :

- Phosgene Process :



Disadvantages : ① phosgene is higely toxic
② requires large amount of $COCl_2$
③ Polycarbonate contamined with Cl impurites.

- Solid state process :



Advantages : ① Phosgene Eliminated
② Higher-quality polycarbonates

④ **Design for Energy Efficiency:** Energy requirements should be minimized Synthetic methods should be conducted at ambient temp. & pressure.

* Energy requirements → minimum
* If heat is required to reflux for a required time, time → minimum
* Use of Catalyst, lowering Eactivation.
* Energy to reaction can be supplied by photochemical means, microwave or sonication.

⑤ **Safer Solvents and Auxiliaries :** Reduce use of unnecessary and pollution causing solvents & Auxiliaries.

* Solvent not cause any pollution and health hazard.
* Rxn → in aqueous phase or solid phase (Best)
* Rxn → without solvent (if possible)
* Use of liquid or supercritical CO_2 should be explored.
* Immobilised solvent : Non Volatile and does not expose humans or the environment to the hazards of that substance.
* Ionic liq : $[Et\,NH_3][NO_3]$
* Clay Zeolits.

Solvents

Preferred	Useable	Undesirable
Water	Cyclohexane	Pentane.

Ethanol	2-MethyTHF	Benzene
1-Butanol	Toluene	Dichloromethane
t-Butanol	Heptain	Pyridine

⑥ **Use Of Renewable feedstocks:** A raw material or feedstock should be renewable rather than depleting whenever technically and economically practical.

* Agricultural or biological products are referred to as renewable starting materials, But cannot be obtained in continuous supply due to crop failure.
* CO_2 & Methane are very abundant and considered as renewable starting material.
* Biofine process.

⑦ **Use of Protecting Groups / Reduce Derivatives:** Unnecessary derivatization (blocking group, protection/deprotection, temporary modification of physical/chemical processes) should be avoided whenever possible.

⑧ **Catalysis:** Catalysts performs transformation without consumed in the rxn and without being incorporation in the final product hence is preferred whenever possible.

Adv.: - Better yeild - selectivity
- Rxn becomes feasible - decrease E_A.
- Minimum Waste product.

⑨ **Design for Degradation:** Chemical products should be designed so that it is degradable.

⊙ DDT bioaccumulate in many plant and animal species and incorporate into the food chain.

* Intsecticides must be biodegradable.
* during degradation the products themselves should not possess any toxic effects or be harmful to human being.
* Functional grps should be susceptible to hydrolysis, photolysis or other cleavage.

⊙ PLA → Polylactic acid

* Manufactured from renewable resources → Corn or Wheat; agricultural waste in future.
* Uses 20-50% fewer fossil fuels than conventional plastics.
* PLA products can be recycled or composted.

(11) Real-time Analysis for Pollution Prevention:

(12) Inherently safer Chemistry for Accident Prevention: