(10) **Design for degradation**

Chemical products should be designed so that at the end of their function they break down into innocuous degradation products and do not persist in the environment. Example: Plastics replaced by biodegradable plastics containing cellulose.

(11) **Real-time analysis for pollution prevention**

Analytical methodologies need to be further developed to allow for real-time, in process monitoring and control prior to the formation of hazardous substances as byproducts. Developing analytical process monitoring are important. The quick detection of harmful substance can help in curative action.

(12) **Inherently safer chemistry for accident prevention** **(M.U. May 2019)**

Substances and the physical form of a substance (solid, liquid or gas) used in a chemical process should be chosen to minimize the potential for chemical accidents, including releases to the environment, explosions, and fires.

5.3 Atom Economy

The concept of Atom Economy was developed by ***Barry Trost***. Any synthetic design s two important goals, namely, reaction efficiency and product selectivity. However, en when a synthetic transformation achieves 100% selectivity to the desired product, a stantial quantity of waste can be generated, if the transformation is not "atom nomical".

Atom Economy is defined as the ratio of the formula weight of the target molecule formula weights of all the starting materials and the reagents. It indicates the intrinsic ency of the desired transformation. Good atom economy indicates that most of the of reactants are transformed into the desired products and only small amounts of ted by-products are formed and hence there are fewer problems of waste disposal or treatment.

tom Economy can be calculated by using the following formula :

$$\% \text{ Atom Economy} = \frac{\textbf{Molecular Weight of product}}{\textbf{Total molecular weight of all the reactants}} \times 100$$

lculation of Atom Economy can be explained by taking the following example:

Preparation of Maleic Anhydride **(M.U. Dec. 2019)**

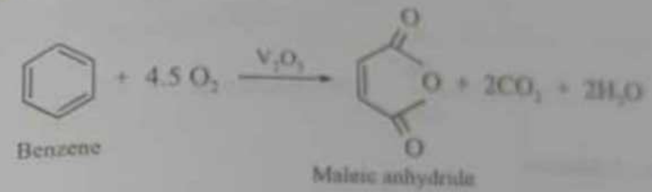
Maleic Anhydride can be prepared by the following three methods

(1) Oxidation of Benzene

(2) Oxidation of Butene

(3) Oxidation of Butane

(1) **Oxidation of Benzene**



$$\underset{\text{Benzene}}{C_6H_6} + 4.5\,O_2 \xrightarrow{V_2O_5} \underset{\text{Maleic anhydride}}{C_4H_2O_3} + 2CO_2 + 2H_2O$$

Molecular weights :-

Benzene, $C_6H_6 = 78$

Oxygen, $O_2 = 32$

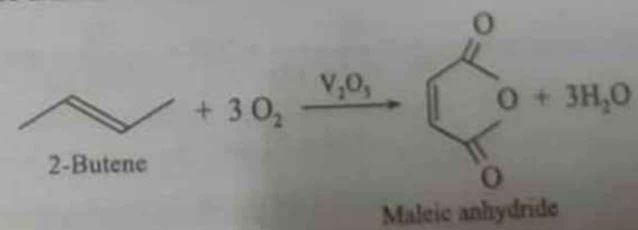
Maleic anhydride, $C_4H_2O_3 = 98$

$$\therefore \quad \% \text{ Atom Economy} = \frac{\text{Molecular weight of maleic anhydride}}{\text{Total molecular weight of benzene and oxygen}} \times 100$$

$$= \frac{98}{78 + (4.5 \times 32)} \times 100 = \frac{98}{78 + 144} \times 100$$

$$= \frac{98}{222} \times 100 = 44.144\,\%$$

(2) **Oxidation of Butene**



$$\underset{\text{Butene}}{C_4H_8} + 3\,O_2 \xrightarrow{V_2O_5} \underset{\text{Maleic anhydride}}{C_4H_2O_3} + 3H_2O$$

Molecular weights :-

Butene, $C_4H_8 = 56$

Oxygen, $O_2 = 32$

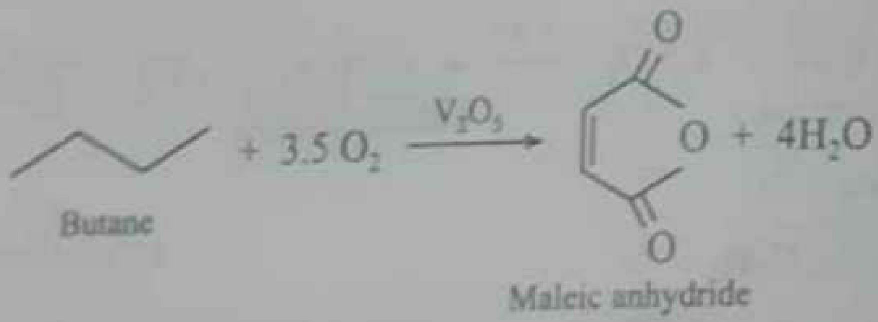
Maleic anhydride, $C_4H_2O_3 = 98$

$$\therefore \quad \% \text{ Atom Economy} = \frac{\text{Molecular weight of maleic anhydride}}{\text{Total molecular weight of butene and oxygen}} \times 100$$

$$= \frac{98}{56+(3\times 32)} \times 100 = \frac{98}{56+96} \times 100$$

$$= \frac{98}{152} \times 100 = 64.474\ \%$$

(3) **Oxidation of Butane**



$$\underset{\text{Butane}}{C_4H_{10}} + 3.5\,O_2 \xrightarrow{V_2O_5} \underset{\text{Maleic anhydride}}{C_4H_2O_3} + 4H_2O$$

Molecular weights :-

Butane, $C_4H_{10} = 58$

Oxygen, $O_2 = 32$

Maleic anhydride, $C_4H_2O_3 = 98$

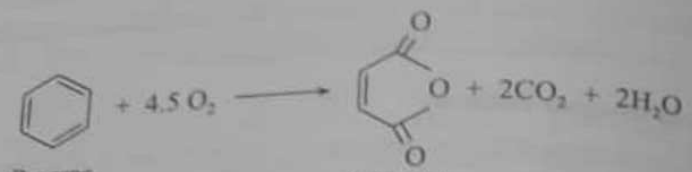
$$\therefore \quad \% \text{ Atom Economy} = \frac{\text{Molecular weight of maleic anhydride}}{\text{Total molecular weight of Butane and oxygen}} \times 100$$

$$= \frac{98}{58+(3.5\times 32)} \times 100 = \frac{98}{58+112} \times 100$$

$$= \frac{98}{170} \times 100 = 57.647\ \%$$

As can be seen, the % atom economy in all the three methods are 44.14%, 64.47% and 57.64% respectively. As the % atom economy is the highest in the second method, i.e. by oxidation of 2-Butene, it is considered to be the greener method and therefore, a better method.

Solution :



Benzene MW = 78   MW = 144   MW = 98

$$\% \text{ Atom Economy} = \frac{\text{MW of product}}{\text{Total MW of reactant}} \times 100$$

$$= \frac{98}{78 + 144} \times 100$$

$$= \frac{98}{222} \times 100$$

$$= 44.1 \%$$

Ans. : % Atom Economy = 44.1 %

Problem 2

Calculate the % Atom economy for the following reaction with respect to Allyl chloride. **(M.U. Dec. 2008, 2011, 2014, 2017; Nov. 2018; May 2017, 2019)**

$$CH_3 - CH = CH_2 + Cl_2 \longrightarrow \underset{\text{Allyl chloride}}{Cl - CH_2 - CH = CH_2} + HCl$$

Solution :

$$\underset{MW = 42}{CH_3 - CH = CH_2} + \underset{MW = 71}{Cl_2} \longrightarrow \underset{\substack{\text{Allyl chloride} \\ MW = 76.5}}{Cl - CH_2 - CH = CH_2} + HCl$$

$$\% \text{ Atom Economy} = \frac{\text{MW of product}}{\text{Total MW of reactant}} \times 100$$

$$= \frac{76.5}{42 + 71} \times 100$$

$$\% \text{ Atom Economy} = \frac{76.5}{113} \times 100$$

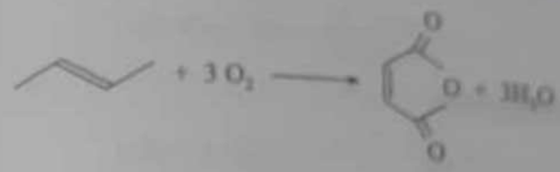
$$= 67.69 \%$$

Ans. : % Atom Economy = 67.69 %

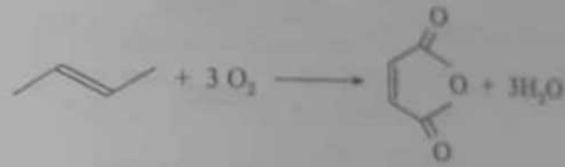
Problem 3

Calculate percentage economy for the following reaction

Synthesis of Maleic Anhydride by oxidation of butane. **(M.U. May 2009; Dec. 2009)**



Solution :



MW = 56   MW = 96   MW = 98

$$\% \text{ Atom Economy} = \frac{\text{MW of product}}{\text{Total MW of reactant}} \times 100$$

$$= \frac{98}{56 + 96} \times 100$$

$$= \frac{98}{152} \times 100$$

$$= 64.5 \%$$

Ans. : % Atom Economy = 64.5 %

Problem 4

Calculate the % Atom economy for the following reactions. **(M.U. May 2011)**

$$CH_3CH = CH_2 + H_2 \xrightarrow{Ni} CH_3CH_2CH_3$$

$$C_6H_6 + CH_3Cl \xrightarrow{AlCl_3} C_6H_5CH_3 + HCl$$

Solution :

(i) $$\underset{MW = 42}{CH_3CH = CH_2} + \underset{MW = 2}{H_2} \xrightarrow{Ni} CH_3CH_2CH_3$$

$$\% \text{ Atom Economy} = \frac{\text{MW of product}}{\text{Total MW of reactant}} \times 100$$

$$= \frac{44}{42+2} \times 100$$

$$= \frac{44}{44} \times 100 = 100\ \%$$

Ans. : % Atom Economy = 100 %

(ii)

$$C_6H_6 + CH_3Cl \xrightarrow{AlCl_3} C_6H_5CH_3 + HCl$$

MW = 78 MW = 50.5 MW = 92

$$\% \text{ Atom Economy} = \frac{\text{MW of product}}{\text{Total MW of reactant}} \times 100$$

$$= \frac{92}{78+50.5} \times 100$$

$$= \frac{92}{128.5} \times 100 = 71.59\ \%$$

Ans. : % Atom Economy = 71.59 %

Problem 5

Calculate the % Atom Economy for the following reaction with respect to acetanilide.

$$\underset{\text{Aniline}}{C_6H_5NH_2} + (CH_3CO)_2O \longrightarrow \underset{\text{Acetanilide}}{C_6H_5NHCOCH_3} + CH_3COOH$$

(M.U. May 2012, 2014)

[Sol]ution :

$$C_6H_5NH_2 + (CH_3CO)_2O \longrightarrow \underset{\text{Acetanilide}}{C_6H_5NHCOCH_3} + CH_3COOH$$

MW = 93 MW = 102 MW = 135

$$\% \text{ Atom Economy} = \frac{\text{MW of product}}{\text{Total MW of reactant}} \times 100$$

$$\% \text{ Atom Economy} = \frac{135}{93+102} \times 100$$

$$= \frac{135}{195} \times 100 = 69.23\ \%$$

[Ans]. : % Atom Economy = 69.23 %

Problem 6

Calculate % atom economy for following reaction.

(M.U. May 2013 Rev.; Nov. 2018)

Solution :

Benzene MW = 78 MW = 71 Chlorobenzene MW = 112.5

$$\% \text{ Atom Economy} = \frac{\text{MW of product}}{\text{Total MW of reactant}} \times 100$$

$$= \frac{112.5}{78+71} \times 100$$

$$= \frac{112.5}{149} \times 100$$

$$= 75.5\ \%$$

Ans. : % Atom Economy = 75.5 %

Problem 7

Calculate percentage atom economy for the following reaction with respect [to] acetophenone.

(M.U. Dec. 2013 Rev., Dec. 2016; May 201[...]

$$\underset{\text{Benzene}}{C_6H_6} + CH_3COCl \xrightarrow{AlCl_3} \underset{\text{Acetophenone}}{C_6H_5COCH_3} + HCl$$

Solution :

$$\underset{\text{Benzene}}{C_6H_6} + CH_3COCl \xrightarrow{AlCl_3} \underset{\text{Acetophenone}}{C_6H_5COCH_3} + HCl$$

MW = 78 MW = 78.5 MW = 120

$$\% \text{ Atom Economy} = \frac{\text{MW of product}}{\text{Total MW of reactant}} \times 100$$

$$= \frac{120}{78 + 78.5} \times 100$$

$$= \frac{120}{156.5} \times 100 = 76.68 \%$$

Ans. : % Atom Economy = 76.68 %

Problem 8

Calculate percentage atom economy for the following reaction with respect to methyl iso-cyanate. **(M.U. May 2015)**

$$\underset{}{CH_3NH_2} + COCl_2 \longrightarrow \underset{\text{Methyl iso-cyanate}}{CH_3-N=C=O} + 2HCl$$

Solution :

$$\underset{\substack{\text{Methyl amine} \\ MW = 31}}{CH_3NH_2} + \underset{MW = 99}{COCl_2} \longrightarrow \underset{\substack{\text{Methyl iso-cyanate} \\ MW = 57}}{CH_3-N=C=O} + 2HCl$$

$$\% \text{ Atom Economy} = \frac{\text{MW of product}}{\text{Total MW of reactants}} \times 100$$

$$= \frac{57}{31+99} \times 100$$

$$= \frac{57}{130} \times 100 = 43.85 \%$$

Ans. : % Atom Economy = 43.85 %

blem 9

Calculate percentage atom economy for the following reaction with respect to maldehyde. **(M.U. Dec. 2015)**

$$\underset{\text{benzaldehyde}}{C_6H_5CHO} + \underset{\text{acetaldehyde}}{CH_3CHO} \xrightarrow{NaOH} \underset{\text{cinnamaldehyde}}{C_6H_5CH = CHCHO} + H_2O$$

on :

$$\underset{\substack{\text{benzaldehyde} \\ MW = 106}}{C_6H_5CHO} + \underset{\substack{\text{acetaldehyde} \\ MW = 44}}{CH_3CHO} \xrightarrow{NaOH} \underset{\substack{\text{cinnamaldehyde} \\ MW = 132}}{C_6H_5CH = CHCHO} + H_2O$$

$$\% \text{ Atom Economy} = \frac{\text{MW of product}}{\text{Total MW of reactants}} \times 100$$

$$= \frac{132}{106 + 44} \times 100$$

$$= \frac{132}{150} \times 100 = 88 \%$$

Ans. : % Atom Economy = 88 %

Problem 10

Calculate percentage atom economy for the following reaction with respect to benzanilide. **(M.U. May 2016)**

$$\underset{\text{aniline}}{C_6H_5NH_2} + \underset{\text{benzoyl chloride}}{C_6H_5COCl} \longrightarrow \underset{\text{benzanilide}}{C_6H_5NHCOC_6H_5} + HCl$$

Solution :

$$\underset{\substack{\text{aniline} \\ MW = 93}}{C_6H_5NH_2} + \underset{\substack{\text{benzoyl chloride} \\ MW = 140.5}}{C_6H_5COCl} \longrightarrow \underset{\substack{\text{benzanilide} \\ MW = 197}}{C_6H_5NHCOC_6H_5} + HCl$$

$$\% \text{ Atom Economy} = \frac{\text{MW of product}}{\text{Total MW of reactants}} \times 100$$

$$= \frac{197}{93+140.5} \times 100$$

$$= \frac{197}{235.5} \times 100 = 83.65 \%$$

Ans. : % Atom Economy = 83.65 %

5.5 Green Fuel - Biodiesel

(M.U. Dec. 2013, 2014, 2016, 2017; May 2013, 2015, 2018,

Biodiesel is a natural and renewable domestic fuel alternative for diesel e made frum vegetable oils, mostly soy and corn. It contains no petroleum, is nonto biodegradable.

This type of fuel burns clean, which results in a significant reduction of the pollutants that contribute to smog and global warming and emits up to 85% fewe causing agents. It is the only alternate fuel approved by the Environmental P Agency (EPA), has passed every Heath-Effects Test of the Clean Air Act and requirements of the California Air Resources Board (CARB).