P.G.SEMESTER-III

CC-XII

Environmental Chemistry and Green Chemistry

Unit-IV Green Chemistry : Def. & Obj.

Topic- Atom Economy in Chemical Synthesis

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Definition

Green chemistry is "the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances"

12 Principles of Green Chemistry

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7. **Maximize atom economy**

What's atom economy ?

ATOM ECONOMY

Barry Trost, Stanford University

"Because an Atom is a Terrible Thing to Waste"

A Measure of the Efficiency of a Reaction

How many of the atoms of the reactant are incorporated into the final product and how many are wasted?

All the designers of chemical processes want to make the maximum amount of product they can from a given raw material.

It is possible to calculate how successful one of these processes is by using the idea of **yield.**

$$\% \text{ Yield} = \frac{\text{Mass of product actually made}}{\text{Maximum mass of product that could be made (theoretical yield)}} \times 100$$

In a chemical synthesis of calcium oxide, calcium carbonate is roasted in an oven. The equation for the reaction is:

$$CaCO_{3(s)} \rightarrow CaO_{(s)} + CO_{2\,(g)}$$

MMr: 100 56 44

The maximum mass of CaO that could be made from 1mol of $CaCO_3$ (=100g) is 56 g

If 50 kg calcium carbonate is used and 21 kg calcium oxide is made, what is the percentage yield of the reaction?

theoretictal yeld = 28g calcium oxide

$$\% \text{ yeld} = \frac{21\text{kg}}{28\text{ kg}} \times 100 = 75\%$$

ATOM ECONOMY

The idea of yield is useful, but from a Green Chemistry and sustainable development perspective, it is not the full picture. This is because yield is calculated by considering only one product.

One of the key principles of Green Chemistry is that processes should be designed so that **the maximum amount of all the raw materials ends up in the product and a minimum amount of waste is produced**

A reaction can have a high percentage yield but also make a lot of waste product. This kind of reaction has a low atom economy.

Both the yield and the atom economy have to be taken into account when designing a green chemical process.

Look again at the reaction you considered

$$CaCO_{3(s)} \rightarrow CaO_{(s)} + CO_{2\,(g)}$$

MMr: **100** **56** **44**

If we split up the formulae, we can look at what happens to each atom in the reaction. The atoms shown below in bold end up in the product we want, the rest do not:

Ca C **O** O O → **Ca O** C O O

Waste box
1C 2O

From the original atoms, one C atom and two O atoms are wasted – they are not in the final,useful product.

Green chemists define atom economy as

$$\textbf{\% Atom Economy} = \frac{\text{FW of atoms utilized}}{\text{FW of all reactant}} \times \mathbf{100}$$

So for this example,

$$\% \text{ Atom Economy} = \frac{56 \text{ (FW CaO)}}{100 \text{ (FW } CaCO_3\text{)}} \times 100$$

%A.E= 56%

ATOM ECONOMY IN A SUBSTITUTION REACTION

This kind of reaction has a low atom economy.

$$CH_3CH_2CH_2CH_2OH + NaBr + H_2SO_4 \rightarrow CH_3CH_2CH_2CH_2Br + NaHSO_4 + H_2O$$

1 2 3 4 5 6

0.0108mole 0.0129 0.0200 0.0108 mole
0.08g **1.33** **2.0** **1.48 g (theoretical yield)**
limiting reagent

Suppose the actual yield is 1.20 g of compound 4.

%yeld= (1,20g/1,48g) x100 = 81%

$$CH_3CH_2CH_2CH_2OH + NaBr + H_2SO_4 \rightarrow CH_3CH_2CH_2CH_2Br + NaHSO_4 + H_2O$$

1 2 3 4 5 6

ATOM ECONOMY TABLE

Reagents Formula	Reagents FW	Utilized Atoms	Weight of Utilized Atoms	Unutilized Atoms	Weight of Unutilized Atoms
1 C_4H_9OH	74	4C,9H	57	HO	17
2 NaBr	103	Br	80	Na	23
3 H_2SO_4	98	——	0	2H,4O,S	98
Total 4C,12H,5O,BrNaS	275	4C,9H,Br	137	3H,5O,Na,S	138

% Atom Economy = (FW of atoms utilized/FW of all reactants) X 100 = (137/275) X 100 = 50%

FW = formula weight

Step-by-step: How to calculate atom economy

Step 1. Write out the balanced equation

Step 2. Calculate the FW of each of the reactants (remember to account for stoichiometric coefficients)

Step 3. Calculate the FW of the product (remember to account for stoichiometric coefficients)

Step 4. Apply the formula

$$\% \text{ atom economy} = \frac{\text{FW of all atoms utilized}}{\text{Total FW of all reactants}} \times 100$$

The students are requested to keep studying and stay tuned till further updates regarding the content .

THANK YOU !

You can mail your subject related queries on…

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