1 - Chemical equations (part 2)

1. **Atom economy**

Just by writing a balanced chemical equation — without relying on additional calculations or data — you can discover features of a reaction. One of these is called **atom economy**. Atom economy is a measurement of **theoretically how wasteful a reaction would be**, and is one of the parameters used to evaluate the eco-friendliness of a chemical process.

Atom economy is defined as a percentage, the molecular mass of desired product relative to the molecular mass of all reagents:

$$\text{Atom economy} = \frac{\text{molar mass of desired product}}{\text{molar mass of reagents}} = \frac{M_{\text{desired product}}}{\sum M_{\text{reagents}}}$$

As an example, water (desired product) could be made by neutralizing hydrochloric acid $HCl_{(aq)}$ with sodium hydroxide $NaOH_{(aq)}$:

$$HCl_{(aq)} + NaOH_{(aq)} \longrightarrow H_2O_{(l)} + NaCl_{(aq)}$$

The atom economy can be calculated as:

$$\begin{aligned}
\text{Atom economy} &= \frac{M_{H_2O}}{M_{HCl} + M_{NaOH}} \times 100\% \\
&= \frac{((2 \times 1.00) + 16.0)}{(1.00 + 35.5) + (23.0 + 16.0 + 1.00)} \times 100\% \\
&= \frac{18}{76.5} \times 100\% \\
&= 23.5\%
\end{aligned} \tag{1}$$

This means that, *even when everything goes right*, over 75% of the mass is going to some unwanted by-product (NaCl in this case).

In industrial processes this means extra mass needs to be hauled to the plant, and extra mass need to be disposed of.

Prerequisite: balancing chemical equations, calculating molar mass.

(a) i. Calculate the atom economy for the reaction $HCl_{(aq)} + KOH_{(aq)} \longrightarrow H_2O_{(l)} + KCl_{(aq)}$, where water is the desired product.

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ii. By comparing the atom economy with that in 1, state and explain which of these process would be more environmentally friendly.

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(b) Calculate the atom economy for producing water in these reactions:

i. $H_2O_{2(aq)} \xrightarrow{c:MnO_{2(s)}} H_2O_{(l)} + O_{2(g)}$

i. ______________

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ii. Combustion of methane $CH_{4(g)}$

ii. ______________

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iii. Neutralization of sulphuric acid with sodium hydroxide

iii. ______________

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iv. Combustion of hydrogen gas $H_{2(g)}$

iv. ______________

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(c) (Return to this and next question after completing yields of reaction (topic 1.3)) Compare and contrast %yield and atom economy.

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(d) State factors *other than atom economy* that should be considered in comparing whether reactions are environmentally friendly.

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2. **Ionic equations**

In reactions with aqueous ionic compounds ($M^+X^-_{(aq)}$), often only either the cation $M^+_{(aq)}$ or the anion $X^-_{(aq)}$ is active in the making or breaking of bonds. The other ion remains unchanged (and is thus called the **spectator ion**).

An example: when $H^+Cl^-_{(aq)}$ reacts with $Na^+OH^-_{(aq)}$ to give water and sodium chloride, a bond is formed between H^+ and OH^-. The sodium Na^+ and chloride Cl^- ions do not change.

In an **ionic equation**, after the balanced equation is written, spectator ions are cancelled out and removed. This helps focus attention on what is chemically important.

e.g. ionic equation for the neutralization reaction above simplies to:

$$H^+_{(aq)} + Cl^-_{(aq)} + Na^+_{(aq)} + OH^-_{(aq)} \longrightarrow H_2O_{(l)} + Na^+_{(aq)} + Cl^-_{(aq)}$$
$$H^+_{(aq)} + OH^-_{(aq)} \longrightarrow H_2O_{(l)}$$

Write ionic equations for:

(a) Reaction of sulphuric acid with sodium hydroxide

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(b) Reaction of nitric acid with potassium hydroxide

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(c) Reaction of copper sulphate $CuSO_{4(aq)}$ with zinc $Zn_{(s)}$ to give zinc sulphate $ZnSO_{4(aq)}$ and copper $Cu_{(s)}$.

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