Atom Economy

A Higher **Atom Economy** Means Less **Waste**

1) Lots of reactions make **more than one product**.
Some of them will be **useful**, but others will just be **waste**.
2) The **atom economy** of a reaction tells you how much of the **mass** of the reactants is converted into **useful products**, and how much is wasted during a reaction.

$$\text{atom economy} = \frac{\text{total } M_r \text{ of desired products}}{\text{total } M_r \text{ of all products}} \times 100$$

3) If a reaction has **100% atom economy** then **all** the atoms in the reactants have been turned into **useful** (desired) **products**. The higher the atom economy, the 'greener' the process.

EXAMPLE: Calculate the atom economy of the reaction to make hydrogen gas from methane and steam: $CH_{4(g)} + H_2O_{(g)} \rightarrow CO_{(g)} + 3H_{2(g)}$.

First identify the useful product, which in this reaction is hydrogen gas.

$$\text{atom economy} = \frac{\text{total } M_r \text{ of desired products}}{\text{total } M_r \text{ of all products}} \times 100$$

$$= \frac{M_r \text{ of } H_2}{(M_r \text{ of } H_2) + (M_r \text{ of CO})} \times 100$$

$$= \frac{3 \times (2 \times 1.0)}{3 \times (2 \times 1.0) + 1 \times (12.0 + 16.0)} \times 100 = \frac{6.0}{6.0 + 28.0} \times 100 = \mathbf{17.6\ \%}$$

High Atom Economy is Better in Industry

1) **Industrial reactions** are designed to be as **cheap** and **green** as possible. Generally, reactions with high atom economies are the **most efficient** processes as there is **minimal waste**.
2) The reactions with the **highest** atom economy are the ones that only have **one product**. These reactions have an atom economy of **100%**.
3) Reactions with low atom economies **use up resources** very quickly. They also make lots of **waste** materials that have to be **disposed** of somehow. That tends to make these reactions **unsustainable** — the raw materials run out and the waste has to go somewhere.
4) For the same reasons, low atom economy reactions aren't usually **profitable**.
Raw materials are **expensive to buy**, and waste products can be expensive to **dispose of**.
5) The best way around the problem is to find a **use** for the waste products or to find a reaction with a **better** atom economy to make the same product.

Atom (Economy) — upgrade to Superior for only £16.99...

1) a) Ethanol can be made from bromoethane in the following reaction:
$CH_3CH_2Br + NaOH \rightarrow CH_3CH_2OH + NaBr$.
What is the atom economy of this reaction?
b) In industry, ethanol is made from ethene and steam using the following reaction:
$CH_2CH_2 + H_2O \rightarrow CH_3CH_2OH$.
Suggest why this reaction is used, rather than the reaction in part a).

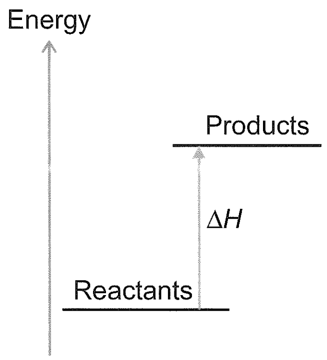
Endothermic and Exothermic Reactions

In an **exothermic** reaction, **heat** energy is **given out** (the room temperature rises).
In an **endothermic** reaction, **heat** energy is **taken** from the surroundings (the room temperature drops).

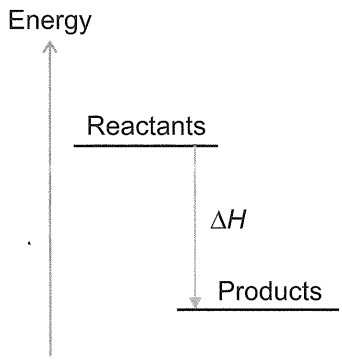
Making and *Breaking* Bonds

1) It takes energy to **break bonds**. When two atoms joined by a bond are **separated**, the energy required to do this must be provided from the surroundings.
2) However, energy is **released** when bonds are made. When two atoms become **joined together** by forming a bond, energy is **released** to the surroundings.
3) In a reaction, if more energy is taken in to break bonds than is given out when bonds are made, the process is **endothermic** — it will take in heat energy. The overall **enthalpy change** of the reaction (ΔH) is **positive**.
4) But, if more energy is given out when bonds are made than is taken in when bonds are broken, the process is **exothermic** — it will give out heat energy. The overall **enthalpy change** of an exothermic reaction (ΔH) is **negative**.

Reactions can be Represented by Energy Level Diagrams



In an **endothermic** reaction, the reactants **take in** energy from the surroundings. The products therefore have **more energy** than the reactants, and ΔH is **positive**.



In an **exothermic** reaction, the reactants **release** energy to the surroundings. The products therefore have **less energy** than the reactants and ΔH is **negative**.

After that I think I need a cup of tea. It'll help improve my energy level...

1) Are the following reactions exothermic or endothermic?
   a) burning coal
   b) sodium hydrogencarbonate + hydrochloric acid (temperature drops)
   c) acid + hydroxide (gets hotter)
   d) methane + steam (cools as they react)
2) a) Draw an energy level diagram for the following reaction:
   $C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$ $\quad \Delta H = -2809$ kJ mol^{-1}
   You should label the products, reactants and enthalpy change on your diagram.
   b) Is the reaction in part a) endothermic or exothermic?

Bond Energy

Average Bond Energy

Bonds between **different atoms** require different amounts of **energy** to break them. When the **same two atoms** bond in the same way, the amount of energy needed is always about the same. The average bond energy values for some common bonds are given below:

C–H 413	C–O 360	C=C 612
O=O 498	H–H 436	C=O 743
C–C 348	O–H 463	

All these values are in kJ mol^{-1}.

The values tell you that:

e.g. It takes 413 kJ of energy to break 1 mole of C–H bonds.

It takes 463 × 2 = 926 kJ to break 1 mole of water (which has 2 O–H bonds per molecule) into oxygen and hydrogen atoms.

743 × 2 = 1486 kJ are released when 1 mole of CO_2 (which has 2 C=O bonds) forms.

Calculating the **Change** in Energy

When a reaction takes place, the change in energy is simply:

sum of energy required to break old bonds – sum of energy released by new bonds formed

EXAMPLE: Calculate the energy change involved when 1 mole of methane burns in oxygen.

The equation for the reaction is: $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

This tells you that 1 mole of methane reacts with 2 moles of oxygen to form 1 mole of carbon dioxide and 2 moles of water.

Step 1: Calculate the energy required to break all of the bonds between the reactant atoms:

4 C–H bonds = 4 × 413 = 1652 kJ

2 O=O bonds = 2 × 498 = 996 kJ

Total = 2648 kJ

Step 2: Calculate the energy released by all the new bonds formed in the products:

2 C=O bonds = 2 × 743 = 1486 kJ

4 O–H bonds = 4 × 463 = 1852 kJ

Total = 3338 kJ

Step 3: Combine the two values to give the overall value for the energy change:

The overall energy change is: 2648 – 3338 = **–690 kJ mol^{-1}**.

The negative sign shows that energy is being released to the surroundings, indicating that this is an **exothermic** reaction. This is expected, since this is a combustion reaction.

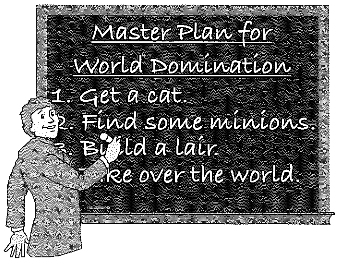
Ian Fleming was like an exothermic reaction — he made lots of Bonds...

1) Calculate the energy change of the following reactions:
(Use the values for the average bond energies given at the top of the page).
   a) burning 1 mole of propane $C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$
   b) burning 1 mole of ethanol $C_2H_5OH + 3O_2 \rightarrow 2CO_2 + 3H_2O$
   c) hydrogenation of 1 mole of ethene $C_2H_4 + H_2 \rightarrow C_2H_6$

Planning Experiments

Make Sure You Plan Your Experiment Carefully

To get accurate and precise results from your experiments, you first need to plan them carefully...



1) Work out the **aim** of the experiment.
2) Identify the **variables** (see below).
3) Decide what **data** to collect.
4) Decide the right **equipment** to use.
5) Plan how to reduce any **risks** in your experiment.
6) Write out a **detailed method**.
7) Carry out **tests** to address the aim of your experiment.

You Need to Control All the Variables

A **variable** is a quantity that might **change** during an experiment, for example temperature. There are two types of variables to know about when carrying out an experiment:

- The **independent variable** is the quantity that you **change**.
- The **dependent variable** is the thing that you measure.

When you plan an experiment you need to work out how you will **control** the variables so that the only one that changes is the one you're investigating — all the others are kept **constant**.

> **EXAMPLE:** Measuring the effect of surface area on reaction rate.
>
> In this experiment, the **independent variable** is the **surface area**, and the **dependent variable** is the **rate** of reaction.
> Everything else, such as temperature and concentration, has to stay exactly the same between different experiments. Surface area is the only variable that you change.

Choose the Right Equipment

You need to think carefully about selecting the right **equipment** for your experiment...

1) The equipment has to be **appropriate** for the specific experiment — for example, in an experiment where you're collecting a **gas** the equipment you use needs to be properly **sealed** so that the gas can't **escape**.
2) The equipment needs to be the right **size**.
3) The equipment needs to be the right level of **sensitivity** — for example, if you want to measure out 4.2 g of a compound, you'll need a balance that measures to at least the nearest 0.1 g, not the nearest gram.

Reduce Risk — and play poker instead...

1) A student is measuring the effect of temperature on the time taken for a lump of magnesium to react completely in a sample of concentrated hydrochloric acid.
   a) What is the dependent variable in the student's experiment?
   b) Name two variables that the student should control to make the experiment a fair test.