#### Chemistry C4 - Chemical Calculations Page 1



### RELATIVE masses, A<sub>r</sub> and M<sub>r</sub>

We cannot actually weigh atoms and molecules because they are TOO SMALL. However we can use RELATIVE masses to help us.

Each atom of an element has a RELATIVE ATOMIC MASS,  $A_r$ 

This is how heavy the atom is compared to a single carbon atom. We assume a carbon atom has a relative mass of exactly 12.

Everything else is compared to this.

Symbols on the periodic table tell us how heavy each element is:

12	40	11 ∢	Atomic Mass A
С	Ca	B	
cantean 6	20	5	

In molecules we can add up the relative masses of EVERY ATOM to give the FORMULA MASS, M<sub>r</sub>

MOLES 1

(Higher)

A MOLE is a numerical term, much like the words PAIR or DOZEN. It relates to a fixed number of something. This fixed number is called the AVOGADRO NUMBER,  $6.02 \times 10^{23}$ A MOLE of a substance will have a mass equal to its formula mass: e.g. if I have  $6.02 \times 10^{23}$  molecules of calcium carbonate,  $CaCO_3$ , it will have a mass of 100.0 g. There is a direct relationship between the number of moles, n, the mass of substance, m and the formula mass of the same substance, M<sub>n</sub> A balanced chemical equation represents this in a different way: it uses symbols and molecular formulae to show the same balance. The numbers of each type of atom at the start and the finish are the same.



# OH NO! THE LAW IS WRONG!

Sometimes it can appear that the law of conservation of mass is wrong! It can appear that the mass of substance has either increased or decreased.

This occurs in OPEN-SYSTEMS where (usually) a gas is allowed to escape or is used in the reaction.

In this reaction one of the products,  $CO_2$ , is a gas and can escape the reaction.

If I weigh the products it will appear that the mass has decreased.

BUT if I could catch and weigh the  $CO_2$  and add it on, I would find the mass does balance! Phew!

### MOLES 3 (Higher)

There are other tricks I can do knowing about moles.

1) LIMITING reagents

If I have LESS of one substance than expected for an equation it will stop the reaction once it has run out. It will **LIMIT** the reaction.

e.g. If I start with only 50 g of  $CaCO_3$  in this reaction, instead of 100 g, it will only use up half the amount of HCl, even if I have more HCl present.

## 2) Working out MOLE ratios for equations

I can work backwards from masses to give the RATIOS by turning masses into moles, using  $n = m/M_r$  then simplifying the ratio of moles.

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Reactants	Products	CHEMICAL VIELDS		
$n = CaCO_{3(aq)} + 2$	$HCl_{(aq)} \rightarrow CaCl_{2(aq)} + CO_{2(g)} + H_2O_{(I)}$	The efficiency of a reaction can be calculated as a <b>CHEMICAL YIELD</b> , which represents the amount of		
c         v         M <sub>r</sub> = 100         M <sub>r</sub>	= 36.5 $M_r$ = 111 $M_r$ = 44 $M_r$ = 18	product <u>actually produced</u> in a reaction compared to the amount that <u>should have been produced</u> this is called the theoretical vield/amount		
<b>CONCENTRATIONS of solutions</b> When a substance is dissolved in a solvent to produce a solution we can calculate the strength of the solution. The substance dissolved is called the solute and the amount of the solute per volume is called the CONCENTRATION. Concentration, c (g/dm <sup>3</sup> )= mass(g)/volume (dm <sup>3</sup> ) If I dissolve 11.1 g of CaCl <sub>2</sub> in 1 dm <sup>3</sup> of water, the concentration c = 11.1/1 = 11.1 g/dm <sup>3</sup> .	CALCULATING theoretical YIELDS Method 1: Simple scaling of the formula masses The equation reads as "100 g of $CaCO_3$ will react to produce 111g of $CaCl_2$ " If I start with half as much $CaCO_3$ , I would expect half as much $CaCl_2$ . If I start with $x$ g of $CaCO_3$ , I should produce $\underline{x} \times 111$ g of $CaCl_2$ 100	Chemical yield = $\frac{\text{amount produced}}{\text{theoretical amount}} \times 100$ theoretical amount E.g. In the reaction above I start with 100 g of $CaCO_3$ this <b>SHOULD</b> produce 111 g of $CaCl_2$ however, it only makes 93.7 g of $CaCl_2$ what is the yield? Yield = <u>93.7</u> × 100 = 84 % <u>111.0</u>		
However if I dissolve 11.1 g of $CaCl_2$ in 0.25 dm <sup>3</sup> , the concentration c = 11.1/0.25 = 44.4 g/dm <sup>3</sup> If the volume is given in different units make sure to convert it into dm <sup>3</sup> first: 11.1 g CaCl <sub>2</sub> dissolved in 200 cm <sup>3</sup> becomes (convert it into dm <sup>3</sup> ) 200/1000 dm <sup>3</sup> = 0.20 dm <sup>3</sup> And concentration c = 11.1/0.20 = 55.5 g/dm <sup>3</sup>	<ul> <li>CALCULATING theoretical YIELDS Method 2: Using moles. This is MORE important when the numbers in front of the reactant and product are NOT the same.</li> <li>a) Calculate the number of moles n of your reactant using n = m/M<sub>r</sub>.</li> <li>b) Use the ratio of the numbers in front of the</li> </ul>	ATOM ECONOMY (atom utilization) The efficiency of a reaction can be calculated in a different way using ATOM ECONOMY. This compares the $M_r$ of USEFUL product as a percentage of the overall $M_r$ of ALL the reactants: Atom economy = $\frac{Mr \text{ useful product}}{Mr \text{ ALL reactants}} \times 100$		
<b>Concentrations HIGHER TIER ONLY</b> Concentrations can also be given in units of moles per dm <sup>3</sup> , written mol/dm <sup>3</sup> or mol dm <sup>-3</sup>	<ul> <li>c) Use the equation of the numbers in from of the reactant and product to calculate the number of moles of product</li> <li>c) Use the equation m = n × M<sub>r</sub> to calculate the expected mass of productthe theoretical yield</li> </ul>	In the example above, if we designate the $CaCl_2$ as 'useful' and the H <sub>2</sub> O and $CO_2$ as 'waste', the atom economy would be: $111 \times 100 = 64 \%$ 100+36.5+36.5		
n = m/M <sub>r</sub> ) then concentration c (mol/dm <sup>3</sup> ) = number of moles (n) /volume (dm <sup>3</sup> )	e.g. How much CaCl $_{\rm 2}$ is produced if I start with 18.25 g of HCl?	VOLUMES of GASES HIGHER TIER ONLY The final calculation we need allows us to convert VOLUMES OF GASES into a number of males		
e.g. If I dissolve 11.1 g of CaCl <sub>2</sub> in 1 dm <sup>3</sup> of water The number of moles of CaCl <sub>2</sub> = 11.1/111 = 0.1 moles And the concentration c = 0.10/1 = 0.10 mol/dm <sup>3</sup> .	Step a) Number of moles of HCl = $18.25/36.5 = 0.5$ Step b) from the equation the ratio of HCl: CaCl <sub>2</sub> is 2:1so there is half the number of moles of CaCl <sub>2</sub> compared to HCln = $0.25$ moles Step c) Mass of CaCl <sub>2</sub> = n × M <sub>r</sub> = $0.25 \times 111 = 27.8$ g CHALLENGEL In this example the HCl is likely to be	Number of moles = volume of gas given molar gas volume The molar gas volume is the volume of any gas at		
As a final example: $55.5 \text{ g } CaCl_2$ dissolved in 2500 cm <sup>3</sup> of water: Number of moles n = m/M <sub>r</sub> = $55.5/111 = 0.5$ mols Volume = 2500 cm <sup>3</sup> = 2500/1000 = 2.5 dm <sup>3</sup> Concentration = $0.5/2.5 = 0.20$ mol/dm <sup>3</sup>	given as a solution with a concentration and a volume used e.g. 250 cm <sup>3</sup> of 1.0 mol/dm <sup>3</sup> solutionyou will need to use your knowledge of concentrations to calculate the number of moles of HCl, then do steps b and c n = c x v = 1.0 x 0.25 = 0.25 moles	pressure. It is a fixed value of 24 dm <sup>3</sup> . In the reaction above 100 g (1 mole) of $CaCO_3$ produces <b>1 mole</b> of $CO_2$ what volume of $CO_2$ is this? Volume of gas = n x molar volume = <b>1</b> x 24 = 24 dm <sup>3</sup>		