Chem Factsheet

September 2000 Number 02

Moles and Formulae

To succeed with this topic you need to:
- be able to find A_r (atomic mass number) values from the Periodic Table
- use a calculator to do basic arithmetic

After working through this Factsheet you will be able to:
- calculate M_r (molecular mass number) from A_r values
- calculate percentage composition by mass for a compound
- calculate moles from grams and grams from moles of a substance
- calculate empirical formulae using a variety of different methods
- convert empirical formulae into molecular formulae

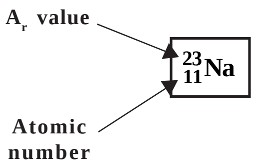
Examination guide

The calculations covered by this Factsheet can appear in nearly every module of the AS and A2 specification. The concepts and methods introduced are the basis of all quantitative chemistry and it is vital you can handle them.

1. Finding M_r (relative molecular mass or formula mass)

The M_r of a compound is found by adding up the relative atomic masses (A_r) of the elements in the compound's formula.

Remember: The A_r value is found from the Periodic Table.



Hint: A_r is always the larger of the two number in the boxes

Example 1: What is the M_r of C_2H_6?

C_2H_6 includes 2 C atoms and 6 H atoms.
So $M_r(C_2H_6) = 2 \times A_r(C) + 6 \times A_r(H)$
(A_r = 12 for C and 1 for H)

$\therefore M_r = (2 \times 12) + (6 \times 1) = 30$

Example 2: What is the M_r of $Ca(NO_3)_2$?

NB: The small 2 outside the brackets multiplies everything inside the bracket - just like in maths.

So $Ca(NO_3)_2$ includes 1 Ca atom, 2 N atoms and 6 O atoms.
So $M_r(Ca(NO_3)_2) = A_r(Ca) + 2 \times A_r(N) + 6 \times A_r(O)$
(A_r = 40 for Ca, 14 for N and 16 for O)

$\therefore M_r = 40 + (2 \times 14) + (6 \times 16) = 164$

2. The percentage composition of a compound

You may be asked to find (for example) the percentage of sodium nitrate that is nitrogen. N.B this is a commonly asked examination question!

Method
Step 1:- find M_r (by totalling A_r values)

Step 2:- find % of an element using:

$$\frac{\text{no. of atoms of element} \times A_r}{M_r} \times 100\%$$

Example: What is the percentage by mass of each of the elements present in C_2H_5Br?

$$M_r(C_2H_5Br) = (12 \times 2) + (1 \times 5) + (80 \times 1) = 109$$

$$\%\,C = \frac{12 \times 2}{109} \times 100 = 22.02\,\%$$

$$\%\,H = \frac{1 \times 5}{109} \times 100 = 4.59\,\%$$

$$\%\,Br = \frac{80 \times 1}{109} \times 100 = 73.39\,\%$$

Check! these should add up to 100%

3. Moles

What is a mole?

A mole of something is just 6.023×10^{23} of it. A mole of hydrogen atoms is 6.023×10^{23} hydrogen atoms, a mole of water molecules is 6.023×10^{23} water molecules - you could even imagine a mole of people or a mole of cars! The number 6.023×10^{23} is called the Avagadro Number - you do NOT have to learn it!

***Exam Hint: -** Be careful what it's a mole of! A mole of hydrogen atoms (H) is not the same as a mole of hydrogen molecules (H_2). A mole of hydrogen molecules contains 2 moles of hydrogen atoms! If a question refers to a mole of an element, it means a mole of **molecules** of that element.*

Why that particular number?

Avagadro's number is chosen to "fiddle" it so that one mole of a substance has mass (in grams) equal to the A_r or M_r of that substance. So as hydrogen atoms have A_r = 1, one mole of hydrogen atoms will have mass one gram. Similarly, as C_2H_6 has M_r = 30, one mole of C_2H_6 will have mass 30 grams. This makes moles easier to work with!

Definition of a mole

The definition of a mole given below probably seems a bit odd, but it is the one that must be given in an exam!

***Definition:** One mole is the amount of substance which contains the same number of particles (atoms, molecules or ions) as there are atoms in 12.00g of ^{12}C*

Calculating with Moles

The important thing is to be able to use the mole in calculations.
The basic equation is:

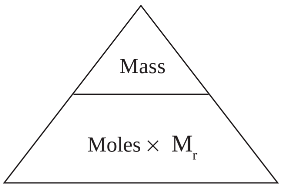
$$\text{Number of moles} = \frac{\text{mass (g)}}{A_r \text{ or } M_r}$$

or rearranged

$$\text{Mass (g)} = \text{moles} \times A_r \text{ or } M_r$$

$$A_r \text{ or } M_r = \frac{\text{mass (g)}}{\text{moles}}$$

Some students find the 'triangle method' useful in remembering and rearranging equations.



You cover up the thing in the triangle you want to find. Then, what you can see tells you the calculation to do. For example, if you want to find moles, cover it up and you are left with mass/M_r

This method can be used for ANY equation that has a fraction on one side and just one thing on the other side. Whatever is on the top of the fraction goes in the top of the triangle.

Here are some examples:

Example 1: How many moles are there in 6g of C?

$$\text{moles} = \frac{\text{mass(g)}}{A_r} \quad (A_r = 12 \text{ for C})$$

$$\therefore \text{ moles} = \frac{6}{12} = 0.5 \text{ moles}$$

Example 2: How many moles are there in 36g of H_2O?

Since M_r is in the formula, we must calculate this first

$$M_r(H_2O) = (1 \times 2) + (16 \times 1) = 18$$

$$\text{moles} = \frac{\text{mass(g)}}{M_r} = \frac{36}{18} = 2 \text{ moles}$$

Example 3: What is the mass of 0.5 moles of H_2S?

$$M_r(H_2S) = (1 \times 2) + (32 \times 1) = 34$$

$$\text{mass(g)} = \text{moles} \times M_r = 0.5 \times 34 = 17 \text{ g}$$

Example 4: 0.2 moles of a metal have a mass of 4.6g.
i) Calculate the element's atomic mass
ii) Suggest an identity for the metal.

$$\text{i) } A_r = \frac{\text{mass(g)}}{\text{moles}}$$

$$= \frac{4.6}{0.2} = 23$$

ii) Looking at the Periodic Table, we see that sodium has an atomic mass of 23, and it is a metal.

***Challenge Question**: Does the metal HAVE to be sodium?*

Answer: No. It is the most likely answer, but isotopes of other metals could have atomic mass 23.

4. Empirical and Molecular Formulas

For <u>calculation</u> purposes there are 2 types of formulae you need to know:

- The **empirical formula (ef)** shows the ratio of the atoms present in their lowest terms i.e. cancelled down to smallest whole numbers.
- The **molecular formula (mf)** shows the actual number of each type of atom present in one molecule.

Finding Empirical Formulae

There are several ways to calculate empirical formulae, and these are shown below in order of increasing difficulty:-

1. Calculating EF from Moles

What is the EF of the compound formed when 6 moles of potassium atoms react with 3 moles of oxygen atoms?

	K:O	
Moles	6 :3	
Simplest ratio	2 :1	(divided by 3)
EF =	K_2O	

2. Calculating EF from Mass

What is the EF of the compound formed when 6g of carbon reacts with 32g of sulphur?

First find moles:

$$\text{moles C} = \frac{6}{12} = 0.5 \quad \text{Moles S} = \frac{32}{32} = 1$$

	C : S	
moles	0.5 : 1	(now divide by 0.5 - the smaller number)
Simplest ratio	1 : 2	

EF =CS_2

3. Calculating EF from Percentage Composition

NB. This is the most commonly examined method of finding EF. The approach is exactly the same as calculating from mass; you treat the percentages as if they are masses. One method of approaching these is using a table, as shown below - but you must use whichever style of presentation you are most comfortable with.

What is the empirical formula for the compound which contains the following elements by percentage composition of mass?
C = 66.67%, H = 11.11%, O = 22.22%

Element	%	A_r	% ÷A_r	Ratio *
C	66.67	12	5.56	5.56 ÷1.39 = 4
H	11.11	1	11.11	11.11 ÷1.39 = 8
O	22.22	16	1.39	1.39 ÷1.39 = 1

EF = C_4H_8O

*To find the ratio column, take the smallest of the %÷A_r values (which is 1.39 here) and divide all the %÷A_r values by it.

4. Calculating EF from Combustion Data

This method is one step up in difficulty from the last example because you have to calculate the masses of the elements first. The combustion products are always oxides. CO_2 and H_2O are the commonest and the following example uses these, although the method can be adapted for others.

Method

Step1:- find mass of the carbon and hydrogen using

$$\text{mass of oxide} \times \frac{\text{no. of atoms of element} \times A_r}{M_r \text{ for oxide}}$$

Find the mass of any other element in the compound by subtraction.

Step 2:- convert mass to moles for each element by dividing by A_r

Step 3:- find the simplest ratio by dividing all the values from step 2 by the smallest of them.

Example: 1g of a compound undergoes complete combustion and produces 2.38g of CO_2 and 1.215g of H_2O. The compound contains only C, H and O. What is its empirical formula?

Step 1: M_r for CO_2 = 44

$$\text{So mass of C} = 2.38 \times \frac{12}{44} = 0.65\text{g}$$

M_r for H_2O = 18

$$\text{So mass of H} = 1.215 \times \frac{2 \times 1}{18} = 0.135\text{g}$$

Mass of O = 1 - 0.65 - 0.135 = 0.215g

Step 2: Moles of C = 0.65 ÷ 12 = 0.054167
Moles of H= 0.135 ÷ 1 = 0.135
Moles of O = 0.215 ÷ 16 = 0.0134375

Step 3: Ratio is:
C : 0.054167 ÷ 0.0134375 = 4
H : 0.135 ÷ 0.0134375 = 10
O : 0.0134375 ÷ 0.0134375 = 1
So the empirical formula is $C_4H_{10}O$

Finding Molecular Formulae

To do this, you need to know (or be able to find) the empirical formula and M_r for the compound.

> Method
> Step 1:- divide M_r by EF formula mass to get scale factor
> Step 2:- multiply EF by scale factor to give MF

Example 1: If the EF = CH_2 and M_r = 42, what is the MF?

$$EF = CH_2 \quad M_r(CH_2) = (12) + (1 \times 2) = 14$$

$$\frac{42}{14} = 3$$

$$\therefore MF = (CH_2) \times 3 = C_3H_6$$

Example 2: 0.24 moles of a compound, containing carbon and hydrogen only, have mass 18.72 grams. On complete combustion, this amount of the compound yields 63.36g of carbon dioxide and 12.96g of water. Find the molecular formula of this compound.

First find the EF. We use the combustion data for this:

$$\text{Mass of C} = 63.36 \times \frac{12}{44} = 17.28\text{g}$$

$$\text{Mass of H} = 12.96 \times \frac{2 \times 1}{18} = 1.44\text{g}$$

Moles of C = 17.28 ÷ 12 = 1.44
Moles of H= 1.44 ÷ 1 = 1.44
So ratio is 1:1 and EF is CH

Now we need M_r in order to find the molecular formula.
We must use the other information in the question:
M_r = mass ÷ moles = 18.72 ÷ 0.24 = 78
M_r (CH) = 13.
78 ÷ 13 = 6
So MF = (CH) × 6 = C_6H_6

Practice Questions

Mole calculations (except for volumetric analysis) make up parts of 'A' level questions. The 13 questions below are designed to give you practice in the different types covered by this Factsheet.

1. Calculating moles of elements (using A_r values)
How many moles are there in each of the following?

(a) 46g Na (b) 12g Mg
(c) 44g Sr (d) 21g Li
(e) 64g S (f) 127g I_2
(g) 64g O_2 (h) 7g Si
(i) 7g N_2 (j) 142g Cl_2
(k) 12.5g of bromine gas (l) 0.787g of neon
(m) 37.9g of fluorine gas (n) 1.89g of potassium
(o) 7.14g of oxygen gas

2. Calculating the mass of element (using A_r values)
What is the mass (in g) of each of the following?

(a) 4 moles A_r (b) 0.5 moles Ca
(c) 0.75 moles Mg (d) 1.5 moles Li
(e) 2 moles Fe (f) 0.5 moles Br_2
(g) 7 moles I_2 (h) 2.5 moles O_2
(i) 3 moles Cu (j) 0.25 moles C
(k) 0.18 moles of fluorine gas (l) 1.75 moles of argon
(m) 0.102 moles of silver (n) 12.5 moles of lead
(n) 3.9 moles of sodium

3. Calculating A_r values from mass and moles
What is the A_r value of the following elements?

(a) 0.27 moles of Pl has a mass of 55.89g
(b) 18g of O_2 contains 0.563 moles
(c) 0.40 moles of S has a mass of 12.8g
(d) 240g of Ca contains 6 moles
(e) 14.80g of Mg contains 0.617 moles

4. Finding relative molecular mass (M_r) from relative atomic masses (A_r)
What is the relative molecular mass of the following?

(a) CO_2 (b) H_2O (c) H_2SO_4
(d) SO_3 (e) CH_4 (f) $(CH_3)_2CO$
(g) C_2H_5OH (h) $MgCO_3$ (i) $Cu(NO_3)_2$
(j) $SiCl_4$ (k) $Na_2CO_3.10\ H_2O$
(l) $CuSO_4.5H_2O$ (m) $CH_3\ (CH_2)_5\ Br$
(n) $Na_2S_2O_3.5H_2O$ (o) Cl_2O_7

5. Calculating moles of compounds (using M_r values)
How many moles are there in each of the following?
(a) 32g SO_2 (b) 90g C_2H_6 (c) 160g SO_3
(d) 22g CO_2 (e) 8g CH_4 (f) 8g MgO
(g) 100g Ca CO_3 (h) 2g CO (i) 14g SiO_2
(j) 80g NO_2 (k) 30.5g $LiNO_3$ (l) 0.87g C_2H_5OH
(m) 6.9g HNO_3 (n) 18g $Na_2CO_3.10H_2O$
(o) 21.55g $CaCl_2$

6. Calculating the mass of compounds (using M_r values)
What is the mass (in g) of each of the following?
(a) 2 moles C_4H_8 (b) 0.33 moles CO
(c) 5 moles CaO (d) 1.5 moles NO
(e) 0.1 moles C_3H_7OH (f) 0.2 moles Na_2O
(g) 0.5 moles $CaCO_3$ (h) 2.7 moles H Cl
(i) 0.7 moles Na Cl (j) 8 moles C_4H_9Br
(k) 4.6 moles H_2SO_4 (l) 0.012 moles C_2H_6
(m) 4 moles ClO_4 (n) 0.25 moles $(CH_3)_2$ I
(o) 0.56 moles $MgCl_2$

7. Calculating M_r values from mass and moles
   What is the M_r value for each of the following compounds?
   (a) 1.0g of compound A contains 0.0208 moles
   (b) 1.5 moles of compound B has a mass of 105g
   (c) 14.8g of compound C contains 0.117 moles
   (d) 7.0g of compound D contains 0.219 moles
   (e) 0.24 moles of compound E has a mass of 13.92g

8. Find the percentage composition by mass of elements in a compound
   What is the percentage composition by mass of each element in the following compounds?
   (a) $SiCl_4$ (b) C_2H_6 (c) Na_2CO_3
   (d) $CaBr_2$ (e) $CuSO_4.5H_2O$

9. Calculating empirical formula from moles
   What is the empirical formula of compounds with the following composition?
   (a) 2 moles Na with 2 moles I
   (b) 0.1 moles K with 0.05 moles O
   (c) 0.5 moles N with 1.5 moles H
   (d) 0.2 moles Mg with 0.4 moles Cl
   (e) 1.2 moles of a carbon oxide contains 0.4 moles of carbon

10. Calculating empirical formula from mass
    What is the empirical formula of compounds with the following composition by mass?
    (a) 12g C with 16g O
    (b) 6g Mg with 4g O
    (c) 46g Na with 80g Br
    (d) 14g N reacting with H to form 17g of compound
    (e) 22g Sr reacting with O to form 26g of compound

11. Calculating empirical formula from percentage composition
    What is the empirical formula of each of the following compounds?
    (a) 80% C, 20%H
    (b) 52.2% C, 13.1% H, 34.7% O
    (c) 40.4% C, 7.9% H, 15.7% N, 36.0% O
    (d) 38.7% C, 9.7% H, 51.6% S
    (e) 40.2% K, 26.9% Cr, 32.9% O
    (f) 85.25% $BaCl_2$, 14.75% water of crystallisation

12. Calculating empirical formula from combustion data
    What is the empirical formula of each of the following compounds?
    (a) Complete combustion of 1.0g of a compound produced 2.99g CO_2 and 1.64g H_2O
    (b) 1.0g of a compound underwent complete combustion and produced 3.035g CO_2 and 1.55g H_2O
    (c) 2.0g of a compound produced 5.86g CO_2 and 3.6g H_2O on complete combustion
    (d) A compound made of carbon, hydrogen and oxygen produced 2.2g CO_2 and 1.2g H_2O when 1.0g of it underwent complete combustion

13. Finding molecular formula from empirical formula and M_r
    What is the molecular formula of the following?

(a)	E.F. = CH	M_r = 72
(b)	E.F. = C_2H_2O	M_r = 42
(c)	E.F. = C_2H_3Br	M_r = 214
(d)	E.F. = CH_2O	M_r = 120
(e)	E.F. = NaO	M_r = 78

Answers

1.	(a) 2	(b) 0.5	(c) 0.5
	(d) 3	(e) 2	(f) 0.5
	(g) 2	(h) 0.25	(i) 0.25
	(j) 2	(k) 0.078	(l) 0.0385
	(m) 2.11	(n) 0.048	(o) 0.223
2.	(a) 160g	(b) 20g	(c) 18g
	(d) 10.5g	(e) 112g	(f) 80g
	(g) 1778g	(h) 80	(i) 193.5g
	(j) 3g	(k) 3.24g	(l) 70g
	(m) 11.02g	(n) 2587.5g	(o) 89.7g
3.	(a) 207	(b) 32	(c) 32
	(d) 40	(e) 24	
4.	(a) 44	(b) 18	(c) 98
	(d) 80	(e) 16	(f) 58
	(g) 46	(h) 84	(i) 188.5
	(j) 170	(k) 286	(l) 249.5
	(m) 123	(n) 248	(o) 183
5.	(a) 0.5	(b) 3	(c) 2
	(d) 0.5	(e) 0.5	(f) 0.2
	(g) 1	(h) 0.071	(i) 0.23
	(j) 1.74	(k) 0.44	(l) 0.019
	(m) 0.11	(n) 0.063	(o) 0.194
6.	(a) 112g	(b) 9.24g	(c) 280g
	(d) 42g	(e) 6g	(f) 12.4g
	(g) 50g	(h) 98.55g	(i) 40.95g
	(j) 1096g	(k) 450.8g	(l) 0.36g
	(m) 398g	(n) 42.75g	(o) 53.2g
7.	(a) 48	(b) 70	(c) 126.5
	(d) 32	(e) 58	

8. (a)	16.57% Si,	83.43% Cl		
(b)	80 % C,	20 % H		
(c)	43.40%Na,	11.32%C,	45.28% O	
(d)	20 % Ca,	80 % Br		
(e)	25.45% Cu,	12.83% S,	4.00 % H,	57.72% O

9.	(a) Na I	(b) K_2O	(c) NH_3
	(d) $MgCl_2$	(e) CO_2	
10.	(a) CO	(b) MgO	(c) Na_2 Br
	(d) NH_3	(e) Sr O	
11.	(a) CH_2	(b) C_2H_6O	(c) $C_3H_7NO_2$
	(d) K_2CrO_4	(e) $BaCl_2 . 2H_2O$	
12.	(a) C_3H_8	(b) C_2H_5	(c) CH_3
	(d) C_3H_8O		
13.	(a) C_6H_6	(b) C_2H_2O	(c) $C_4H_6Br_2$
	(d) $C_4H_8O_4$	(e) Na_2O_2	

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