CHEQ 1094 FORMULAS

1. INFORMATION FROM A FORMULA

Consider the formula $CaSO_4$. The information contained in that formula can be expressed in several ways. Since $CaSO_4$ is ionic, the formula gives the simplest whole number ratio of the atoms of Ca, S and O in the compound. It also gives the **number** of atoms of Ca, S and O in one **formula unit** of $CaSO_4$. Since a mole is a fixed number, the formula also gives the simplest whole number ratio of the moles of Ca, S and O in the compound **and** the number of moles of Ca, S and O in one **mole** of $CaSO_4$. We can calculate the mass ratio by multiplying the number of atoms (or moles) of each element by its atomic weight (or molar mass). This mass ratio can also be expressed as a percentage by mass. These ratios are set out below.

1. **Atom ratio**:	1 Ca atom	:	1 S atom	:	4 O atoms
2. **Mole ratio**:	1 mole Ca atoms	:	1 mole S atoms	:	4 moles O atoms
3. **Mass ratio**:	40.1 g Ca	:	32.1 g S	:	4 x 16.0 g O
4. **Mass percent**:	29.4% Ca	:	23.6% S	:	47.0% O

For molecular compounds, the molecular formula gives the actual number of atoms of each element in one molecule of the compound. Consider a compound of molecular formula $C_4H_8O_2$ (such as ethyl acetate used as nail polish remover). This formula can be interpreted in terms of atom ratio, mole ratio, mass ratio or mass percent as for the ionic compound $CaSO_4$ above. However, a compound of molecular formula C_2H_4O will have the same atom ratio, mole ratio, mass ratio or mass percent as $C_4H_8O_2$ because $C_4H_8O_2$ is $(C_2H_4O)_2$. We say that these compounds ($C_4H_8O_2$ and C_2H_4O) have different molecular formulas but the same **empirical** formula (C_2H_4O). The empirical formula of a molecular compound is the simplest whole number ratio of the atoms of the different elements. Thus, the compounds $C_6H_{12}O_6$, $C_5H_{10}O_5$ and $C_4H_8O_4$ all have the same empirical formula (CH_2O). If the formula is not divisible by a whole number to give a whole number ratio, its molecular formula is its empirical formula. Examples are $C_9H_8O_2$, $C_4H_6O_3$, etc.

The mass ratio (and hence mass percent) of a compound can be obtained from its mole ratio of its elements and the atomic weights of its elements. Hence, one can work backwards from a mass ratio (including mass percent) to a mole ratio using the atomic weights of the elements.

2. EMPIRICAL FORMULAS

(a) A compound was found to contain 28.83% magnesium, 14.22% carbon and 56.94% oxygen. Calculate the formula of the compound.

Solution:
First, check to see that the sum of the percentages = 100
28.83 + 14.22 + 56.94 = 99.99 (= 100 within experimental error)
Percentages are **mass** percentages. If we consider 100 g of the compound, the percentages are the masses, in grams, of the elements in the compound and represent the **mass ratios** of the elements. Since a formula is an **atom ratio** which is equal to the **mole ratio** of atoms of the elements in the compound, conversion of the mass ratio to the mole ratio and expressing the mole ratio as a **whole number ratio** gives the formula of the compound.

	Mg	C	O
mass (g)	28.83	14.22	56.94
mole ratio	$\frac{28.83}{24.31}$	$\frac{14.22}{12.01}$	$\frac{56.94}{16.00}$
=	1.186	1.184	3.559
divide by smallest (1.184) (to get whole numbers)	1.002	1	3.006

Within experimental error, this ratio is 1 : 1 : 3 and the formula is $MgCO_3$.

The process used above involved the following steps:
1. Use percentages as mass ratio
2. Convert masses to moles
3. Divide by the smallest
4. Round off to 3 significant figures

Where the percentages of all but one of the elements are given, the percentage of that element can be found by difference.

(b) A compound containing K, N and O was found to be 38.7% K and 13.9% N. Calculate the formula of the compound.

(c) Thermal decomposition of 1.9025 g of an oxide of mercury gave 1.8296 g of mercury. Calculate the formula of the oxide. (N.B.: It is not necessary to calculate the **percentage** of each element; any mass ratio can be converted into a mole ratio)

(d) Heating 0.4725 g of iron in the presence of an excess of pure oxygen gave 0.6758 g of a compound. Calculate the formula of the compound.

Mole ratios obtained in calculating formulas may involve only whole numbers, as in examples (a) to (c), or may involve the fraction $\frac{1}{2}$, as in example (d). Many other fractions may be involved in complicated formulas, but in this course only the fractions $\frac{1}{2}$, $\frac{1}{4}$, $\frac{3}{4}$, $\frac{1}{3}$ and $\frac{2}{3}$ will be met. In (d), we saw that we had to multiply $1\frac{1}{2}$ (1.5) by 2 to get a whole number ratio. We can therefore add another step to the generalized calculation of formulas:

5. If step 4 does not give whole numbers, multiply $\frac{1}{2}$ (.5) by 2, $\frac{1}{4}$ (.25) and $\frac{3}{4}$ (.75) by 4, and, $\frac{1}{3}$ (.33) and $\frac{2}{3}$ (.67) by 3.

(e) A compound contained 81.7% carbon and 18.3% hydrogen. Calculate the empirical formula of the compound.

(f) The hormone melatonin is 67.22% C, 6.94% H, 12.06% N and 13.78% O. Calculate the empirical formula of melatonin.

3. MOLECULAR FORMULAS

Formaldehyde, CH_2O, and the sugar ribose, $C_5H_{10}O_5$, have different molecular formulas but each has a 1:2:1 ratio of C:H:O [ribose is $5(CH_2O)$] and hence they both have the same empirical formula, CH_2O. A mass ratio can only give an empirical formula, not a molecular formula. To calculate a molecular formula from an empirical formula, the molecular weight (MW ≡ molar mass, MM) **must** be known. An empirical formula, as any formula, has a formula weight which we can call the empirical formula weight (EFW). The ratio MW/EFW = n must be a whole number and n(empirical formula) = molecular formula.

Example: The sugar D-*manno*-heptulose, isolated from the avocado pear, has an empirical formula of CH_2O and a molar mass of about 205(±7) g/mole. Calculate the molecular formula.

Solution: EFW of CH_2O = [12 + (2x1) + 16] = 30

n = 205/30 = 6.83 $\qquad$ n = 7 (must be a whole number)

molecular formula is $7(CH_2O) = C_7H_{14}O_7$

(a) The empirical formula of dry cleaning fluid, perchloroethylene (PCE), is CCl_2. The molar mass of PCE is 166 g/mole. Calculate the molecular formula of PCE.

(b) Eugenol, the major component of clove oil, is used as a dental analgesic and contains only carbon, hydrogen and oxygen. Eugenol is 73.14% C and 7.38% H and has a molar mass of about 160 g/mole. Calculate the empirical formula of eugenol and **then** its molecular formula.

4. HYDRATES

We can also use the mole ratio approach for calculating the formula of a hydrate. The formula $CuSO_4 \cdot 5H_2O$ means that the mole ratio of H_2O to $CuSO_4$ is 5:1. For a hydrate where the number of moles of water per mole of compound is not known, the mass ratio of water to compound must be found by experiment and then converted into a mole ratio.

(a) When 3.7200 g of $Ni(NO_3)_2 \cdot nH_2O$ was heated to drive off water, a 2.3372 g residue of $Ni(NO_3)_2$ was obtained. Calculate the value of n. (*Ans*. 6)

(b) A hydrate of iron(II) phosphate [$Fe_3(PO_4)_2 \cdot nH_2O$] was found to be 28.74% water. Calculate the value of n. (*Ans*. 8)

(c) When 0.8655 g of $MSO_4 \cdot 7H_2O$ was heated to drive off water, a 0.4227 g residue of MSO_4 was obtained. Calculate the atomic weight of M and hence identify M.
(Hint: Use FW = grams/moles or algebra)(*Ans*. Mg)