MOLECULAR FORMULA AND EMPIRICAL FORMULA

Molecular Formula is a formula indicating the actual number of atoms of each element making up a molecule. The molecular formula must accurately state the exact number of atoms of all of the elements in one molecule of the substance.
Empirical formula is the formula giving the simplest ratio between the atoms of the elements present in a compound. You must find the ratio of atom to atom in a molecule, and then reduce it.
The formula for ionic compounds is an empirical formula.
A molecular formula is a whole number multiple of an empirical formula.
Converting to empirical formula from molecular formula is more difficult than vice versa.

Converting Molecular Formula to Empirical Formula

1. Determine the molecular formula. If the molecular formula is written structurally, then convert it to standard form (Example 2).
2. Divide the entire equation by the largest whole number that all subscripts are divisible by,
3. Write the new equation.

Example 1: Hydrogen Peroxide
Step 1: Molecular Formula is H_2O_2
Step 2: All subscripts are divisible by 2
Step 3: Empirical Formula is HO

Example 2: Glucose
Step 1: Molecular Formula is $C_6H_{12}O_6$
Step 2: All subscripts are divisible by 6
Step 3: Empirical Formula is CH_2O

Creating an Empirical Formula from Mass or Percent Composition

From Percent Composition:
Step 1: Create a chart with six columns and a number of rows equal to the number of elements in the compound.
Step 2: Write the elements in the first column.
Step 3: Write the percent composition of each element in the second column.
Step 4: Using the percent composition as the mass, divide each by the molecular mass of the respective element.
Step 5: Divide each of those numbers by the smallest of the numbers in that column to reduce the ratio. If one or more numbers in the ratio is still distant from a whole number, try multiplying the entire ratio by a whole number. If the number is close, then round it to the nearest whole number. Each one of the numbers is the subscript for the corresponding element.

Example 1: Determine the empirical formula for a compound containing 74.0% carbon, 8.65% hydrogen, and 17.3% nitrogen by mass.

C	74.0%	74.0 g / 12.0 g	6.16 / 1.24	4.96	5
H	8.65%	8.65 g / 1.01 g	8.56 / 1.24	6.90	7
N	17.3%	17.3 g / 14.0 g	1.24 / 1.24	1	1

Therefore the empirical formula is C_5H_7N

From Mass:

Follow the same procedure as fir Percent Composition but first divide the mass of each element by the mass of the total sample. The quotient is the percent composition.

Example 1: A 9.2 g sample of a compound is 2.8 g of nitrogen and 6.4 g of oxygen. Find the empirical formula of the compound.

N	2.8 g / 9.2 g	30%	30 g / 14 g	2.143 g / 2.143 g	1	1
O	6.4 g / 9.2 g	70%	70 g / 16 g	4.375 g / 2.143 g	2.04	2

Therefore, the empirical formula is NO_2.

<u>Creating a Molecular Formula from an Empirical Formula and Molecular Mass</u>

Step 1: Determine the molecular mass in grams.

Step 2: Divide the molecular mass of the compound by the molecular mass (g) of the empirical formula

Step 3: Round the quotient to the closest integer.

Step 4: Multiply the rounded number by all the subscripts using the product as the new subscripts.

<u>Example 1</u>: A compound has an empirical formula of CH2 and a molecular mass of 42 g. Determine its molecular mass.

Step 1: Carbon = 12 + Hydrogen = 2 (1.01)

Molecular Mass (g) = 14.02

Step 2: 2.42 / 14.02 = 2.999

Step 3: 3

Step 4: CH2 * 3 = C_3H_6

Empirical and Molecular Formula Calculations

Empirical formula is the smallest whole number ratio of moles of each element in a compound.

$CaCl_2$ --> there is 1 mole of calcium for every 2 moles of chlorine

Level 1 Simple Empirical formula questions

What is the empirical formula of the following compounds? (so reduce the formula if you can)

molecular formula	empirical formula
C_2H_4	CH_2
$C_{11}H_{22}O_{11}$	CH_2O
H_2O	H_2O
$C_{25}H_{50}$	CH_2

Level 2 Empirical Formula Calculation Steps

Step 1 If you have masses go onto step 2.

If you have %. Assume the mass to be 100g, so the % becomes grams.

Step 2 Determine the moles of each element.

Step 3 Determine the mole ratio by dividing each elements number of moles by the smallest value from step 2.

Step 4 Double, triple … to get an integer if they are not all whole numbers

Molecular Formula (additional steps)

The question should have included a molecular mass.

Step 5 Determine the mass of your empirical formula

Step 6 Divide the given molecular mass by your E.F. mass in step 5

Step 7 Multiply the atoms in the empirical formula by this number

Examples-Caffeine has an elemental analysis of 49.48% carbon, 5.190% hydrogen, 16.47% oxygen, and 28.85% nitrogen. It has a molar mass of 194.19 g/mol. What is the molecular formula of caffeine?

(Hint-Save the molar mass 194.19g/mol until the end)

49.48% C, 5.190%H, 16.47% O and 28.85% N

Step 1 Mass is 100% so % becomes grams

49.48g C, 5.190gH, 16.47g O and 28.85g N

Step 2 determine the moles of each element

49.48g C x (12.0 g C / mole) = 4.123moles C
5.190g H x (1.0 g H / mole) = 5.190 moles H
16.47g O x (16.0 g O / mole) =1.029moles O
28.85g N x (14.0 g N / mole) = 2.061 moles N

Step 3 determine the mole ratio by dividing each elements number of moles by the smallest

Dividing by the smallest (1.029) we get

C: 4.123 / 1.029 = 4.007
H: 5.190 / 1.029 = 5.044
O: 1.029 / 1.029 =1.000
N: 2.061 / 1.029 = 2.002

Step 4 Double, triple .. to get an integer is they are not all whole numbers

The values are all really close to whole numbers.

Empirical Formula= $C_4H_5ON_2$

Example- Molecular Formulas (Steps 5-7)

It has a molar mass of 194.19 g/mol.

Step 5 After you determine the empirical formula, determine its mass.

Empirical Formula= $C_4H_5ON_2$

(4 carbon x 12.0) + (5 hydrogens x1.0) + (1 oxygen x 16.0) + (2 nitrogen x 14.0) =97.0g/mol

Step 6 Determine how many times greater the molecular mass is compared to the mass of the empirical formula.

molecular mass/ empirical formulas mass

194.19g/mol / 97.0g/mol = 2

Step 7 Multiply the empirical formula by this number

2x $C_4H_5ON_2$ =$C_8H_{10}O_2N_4$

better==> $C_8H_{10}N_4O_2$

***note: If step 6 does not work out to be a whole number your empirical formula is wrong or your teacher screwed up