Empirical versus Molecular Formulas

The empirical formula is the lowest whole number ratio of the elements in a compound.

The molecular compound is the actual whole number ratio of elements in a compound, but is not necessarily the lowest whole number ratio.

Compound	Empirical formula	Molecular formula
H_2O	H_2O	H_2O
octane	C_4H_9	C_8H_{18}

The formulas for all ionic compounds are always empirical formulas because that's how an ionic compound gets together - the lowest whole number ratio of ions.

2. Finding Empirical Formula

To find the empirical formula of a compound, you need to know the percentage composition and work from there. Here are the steps involved:

- convert the percentage to a mass
- convert mass to moles
- divide each mole value by the lowest of the mole values
- multiply all mole values by a factor to convert them into whole number - if necessary

Example:

A prospector finds a rock that may contain rutile, an ore of titanium. A crystal was analyzed found to be 59.94 % titanium and 40.06% oxygen by mass. Determine the empirical formula for the crystal.

Step One:
Assume 100 g and use your percentage compositions to determine the mass of each element

m of titanium = 100.0 g x 59.94 % = 59.94 g
m of oxygen = 100.0 g x 40.06% = 40.06 g

Step Two:
Use the mole formula to convert each mass to moles

$$n \text{ of titanium} = \frac{m}{M} = \frac{59.94\ g}{47.88\ g/mol} = 1.252\ mol$$

$$n \text{ of oxygen} = \frac{m}{M} = \frac{40.06\ g}{16.00\ g/mol} = 2.504\ mol$$

Step Three:
Find a ratio of mole values by dividing the larger mole value(s) by the smallest mole value

$$\text{titanium } \frac{1.252}{1.252} = 1$$

$$\text{oxygen } \frac{2.504}{1.252} = 2$$

Since the ratio came out in whole numbers, the empirical formula is TiO_2

They don't always come out to whole numbers, which adds an extra step, as in this example:

Example: Determine the empirical formula of a compound that is 74.39% gallium and 25.61% oxygen.

m of gallium = 100.0 g x 74.39 % = 74.39 g
m of oxygen = 100.0 g x 25.61% = 25.61 g

$$n \text{ of gallium} = \frac{m}{M} = \frac{74.39\ g}{69.72\ g/mol} = 1.067\ mol$$

$$n \text{ of oxygen} = \frac{m}{M} = \frac{25.61\ g}{16.00\ g/mol} = 1.601\ mol$$

$$\text{gallium } \frac{1.067}{1.067} = 1 \qquad \text{oxygen} = \frac{1.601}{1.067} = 1.5$$

Since 1.5 is not a whole number, we multiply both by a factor until they are both whole, so in this case if we doubled them, we would make a whole number ratio of Ga_2O_3

There's a rhyme you can use to help you remember the steps:

percent to mass
mass to mole
divide by small
multiply 'til whole

Now try these to practice:

Determine the empirical formula of galena, a lead ore that is 76.37 % lead and 23.63 % sulfur.

Determine the empirical formula of magnetite, an iron ore that is 72.36 % iron and 27.64 % oxygen.