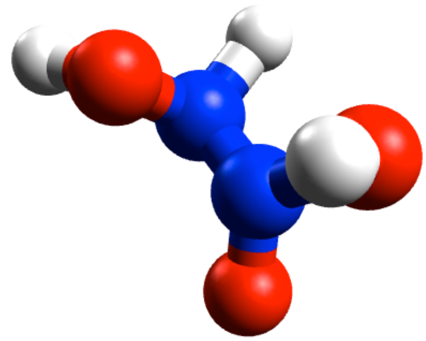
How to Calculate a Molecular Formula



The molecular formula is the blueprint of a molecule. Formulas like C_6H_6 or $C_3H_5NO_2$ tell anyone who reads how many of each atom is contained in a molecule. Determining the molecular formula is an important step to understanding any substance.

To calculate the molecular formula you need the ratio of elements in the compound and the molar mass of that compound.

The ratio of elements can be given as the empirical formula or it might be represented as the percent composition by weight (you can always get the empirical formula from the percent composition).

Example: A compound formed from only nitrogen and oxygen is found to be 30.4457% N and 69.5543% O, the molar mass of the compound is 138.0 g/mol.

Step One: Determine the Empirical Formula

$$30.4457 \text{ grams of N} \times \frac{1 \text{ mol N}}{14.01 \text{ grams N}} = 2.173 \text{ mol N}$$

$$69.5543 \text{ grams of O} \times \frac{1 \text{ mol O}}{16.00 \text{ grams O}} = 4.347 \text{ mol O}$$

$$2.173 \text{ mol N} \times \frac{1}{2.173 \text{ mol}} = 1$$

$$4.347 \text{ mol O} \times \frac{1}{2.173 \text{ mol}} = 2$$

the ratio of N atoms to O is 1:2
the empirical formula is NO_2

The percent composition tells you how much of any sample of the compound is made of each element. For simplicity just pick a sample of about 100 grams--then it's easy to see how many grams of each element are in the sample. If the sample is 100.000 and it's 30.4457% N, then 30.4457 grams of it is Nitrogen.

Next find out how many moles of each element are in those grams of each element. To do this, just divide the number of grams by the atomic mass of the corresponding element.

The total number of moles of each element gives you the ratio of atoms of each element. The simplest way to see what that ratio is, is to divide each number of moles by the smallest number of moles. You won't always get a whole number ratio. Sometimes it will be 1:2 or 1:5, but sometimes it might be one and a half to two. If you get numbers with a simple fraction, multiply the ratio by the smallest number that will give you a whole number ratio.

$$2.459 \text{ mol P} \times \frac{1}{2.459 \text{ mol}} = 1$$

$$3.279 \text{ mol S} \times \frac{1}{2.459 \text{ mol}} = 1.333$$

if the ratio of P atoms to O atoms is 1 : 1.333
multiply both numbers by 3 to get whole numbers
the ratio becomes 3 : 4
the empirical formula is P_3S_4

Step Two: Use the Empirical Formula and Molar Mass to Determine the Molecular Formula

$$1 \text{ N} = 1 \times 14.01 = 14.01$$
$$2 \text{ O} = 2 \times 16.00 = 32.00$$
$$46.01$$
$$138.0 \div 46.01 = 3$$

therefore there are 3 NO_2 units in the molecule, that means the total molecular formula is:

$3 \times NO_2 = N_3O_6$

Once you know what the empirical formula for the compound is, you can calculate the weight of a single formula unit. Example, the formula unit of NO_2 weighs 46.01 grams/mol.

Divide the molar mass of the compound by the formula weight of single empirical unit to find out how many empirical units are in each molecule. Example, if there molar mass indicates there are three NO_2 units in the molecule, the molecular formula is N_3O_6.