

The Mole and Chemical Formulas

A **mole** (also known as Avogadro's Number) is the number that is used in making calculations involving atoms and molecules. Given the relatively microscopic size of the particles, it would be rather difficult (read: utterly pointless) to calculate amounts in terms of numbers of atoms. So, we use the mole.

A mole, (mol for short) is equal to (all together now) **6.022×10^{23}** atoms or molecules.

The **atomic mass** given for an element on the periodic table measured out in grams is equal to one mole of atoms of that element.

Thus, the **Molar Mass (MM)** of elements and compounds is the mass, in grams, equal to the atomic and formula masses of those elements and compounds. The unit of Molar Mass is **grams/mole**.

Empirical and Molecular Formulas

Believe it or not, there is more than one kind of chemical formula (insert a sharp gasp of surprise here). Judging from the heading of this section, they would be **empirical** and **molecular** formulas. Empirical formulas give the *lowest whole number ratio* of the atoms in a compound, whereas the molecular formula gives the *exact composition* of one molecule.

Empirical	Molecular
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HO	H ₂ O ₂
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CH	C ₂ H ₂
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CH	C ₆ H ₆
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NO	NO
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NO ₂	N ₂ O ₄
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Empirical formulas can be calculated using experimental data:

- Given that a certain compound is 69.58% Ba, 6.090% C and 24.32% O, calculate the empirical formula of this compound.
- Assume that you have 100.00 g of the compound:
 - 69.58% Ba = 69.58 g Ba
 - 6.090% C = 6.090 g C
 - 24.32% O = 24.32 g O
- Convert the mass of each element to moles of that element:
 - Ba = $(69.58 \text{ g Ba})(1 \text{ mol Ba}/137.3 \text{ g Ba}) = 0.5068 \text{ mol Ba}$
 - C = $(6.090 \text{ g C})(1 \text{ mol C}/12.01 \text{ g C}) = 0.5071 \text{ mol C}$
 - O = $(24.32 \text{ g O})(1 \text{ mol O}/16.00 \text{ g O}) = 1.520 \text{ mol O}$
- Divide through each value by the smallest number of moles to get a 1 : 1.001 : 2.999 ratio, which rounds off nicely to give the formula BaCO_3

Molecular formulas can be calculated using empirical formulas:

- Given that the empirical formula of a compound is CH and the molar mass is 104 g/mol, calculate the molecular formula.

$$\begin{aligned}\text{mass of C} &= 12.0 \text{ g/mol} \\ \text{mass of H} &= 1.01 \text{ g/mol} \\ \text{empirical formula mass} &= 13.0 \text{ g/mol}\end{aligned}$$

- to find the number of CH units in the compound:
- # CH units = $(104 \text{ g/mol})(1 \text{ mol}/13.0 \text{ g}) = 8.00$
- Molecular formula = $8(\text{CH})$ or C_8H_8

I. Calculating Molar Mass

1. multiply atomic mass of each element by number of atoms of that element in the formula (shown by the subscript)
2. find the sum of all the atomic masses --this is formula mass (unit is a.m.u.)
3. express formula mass in grams (unit is g/mol). This is the **Molar Mass**.

II. Calculating % Composition (from formula)

- calculate formula mass
- divide the total atomic mass of each element by the formula mass and multiply by 100

III. Calculating % Composition (from masses of each element)

1. divide the mass of each element by the total mass of the compound and multiply by 100

IV. Calculating Empirical Formula (from % Composition)

1. convert % of each element to grams based on 100 grams of the compound
2. multiply grams of each element by 1/molar mass that element
3. compare ratio of moles of each element and divide each by the smallest
4. if result in step 3 gives a ratio with decimal equivalent to 1/4, 1/3, 1/2, 2.3, 3/4 instead of whole numbers, convert to the fraction and multiply all ratios by the denominator or the fraction

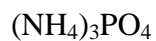
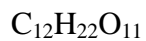
V. Calculating Empirical Formula (from experimentally determined masses)

1. multiply the mass of each element (in grams) by 1/molar mass of that element
2. continue with steps 3 & 4 from IV above.
[Example](#)

VI. Finding Molecular Formulas (when molar mass is known)

1. calculate the empirical formula
2. use the equation : (empirical formula mass)x = molar mass
3. find value for x: $x = \text{molar mass} / \text{empirical formula mass}$
4. multiply each subscript in empirical formula by value for x

1. Calculate the molar masses for each formula using paper and pencil, then check your answer using the Java applet located below. It won't do you any good if you get the answers from the applet. You need to practice calculating them yourself, because the applet won't be available on a test.



Calculating Molarity

The properties and behavior of many solutions depend not only on the nature of the solute and solvent but also on the concentration of the solute in the solution. Chemists use many different units when expressing concentration; however, one of the most common units is **molarity**. Molarity (M) is the concentration of a solution expressed as the number of moles of solute per liter of solution:

$$\text{Molarity (M)} = \frac{\text{moles solute}}{\text{liters solution}}$$

For example, a 0.25 M NaOH solution (this is read as 0.25 molar) contains 0.25 moles of sodium hydroxide in every liter of solution. Anytime you see the abbreviation M you should immediately think of it as mol/L.

In order to calculate the molarity of a solution, you need to know the number of moles of solute and the total volume of the solution.

To calculate molarity:

1. Calculate the number of moles of solute present.
2. Calculate the number of liters of solution present.
3. Divide the number of moles of solute by the number of liters of solution.

Instead of calculating the moles of solute and liters of solution present individually, you can also string all the calculations together in one problem:

1. Divide the amount of solute by the volume of solution (regardless of the initial units given).
2. Use dimensional analysis to convert the amount of solute to moles of solute.
3. Use dimensional analysis to convert the volume of solution to liters of solution (if necessary).

The following example will illustrate both methods.

Example: What is the molarity of a solution prepared by dissolving 15.0 g of sodium hydroxide in enough water to make a total of 225 mL of solution?

Method 1:

- Calculate the number of moles of solute present.

$$\begin{aligned}\text{mol NaOH} &= \frac{15.0 \text{ g NaOH}}{40.0 \text{ g NaOH}} \times \frac{1 \text{ mol NaOH}}{1} \\ \text{mol NaOH} &= 0.375 \text{ mol NaOH}\end{aligned}$$

- Calculate the number of liters of solution present.

$$\begin{aligned}\text{L soln} &= \frac{225 \text{ mL}}{1000 \text{ mL}} \times \frac{1 \text{ L}}{1} = 0.225 \text{ L soln}\end{aligned}$$

- Divide the number of moles of solute by the number of liters of solution.

$$\begin{aligned}M &= \frac{0.375 \text{ mol NaOH}}{0.225 \text{ L soln}} = 1.67 \text{ M NaOH}\end{aligned}$$

Method 2:

- Divide the amount of solute by the volume of solution (regardless of the initial units given).

$$\begin{aligned}M &= \frac{15.0 \text{ g NaOH}}{225 \text{ mL soln}}\end{aligned}$$

- Use dimensional analysis to convert the amount of solute to moles of solute.

$$\begin{aligned}M &= \frac{15.0 \text{ g NaOH}}{225 \text{ mL soln}} \times \frac{1 \text{ mol NaOH}}{40.0 \text{ g NaOH}}\end{aligned}$$

- Use dimensional analysis to convert the volume of solution to liters of solution (if necessary).

$$\begin{aligned}
 M &= \frac{15.0 \text{ g NaOH}}{225 \text{ mL soln}} \times \frac{1 \text{ mol NaOH}}{40.0 \text{ g NaOH}} \times \frac{1000 \text{ mL soln}}{1 \text{ L soln}} \\
 M &= 1.67 \frac{\text{mol NaOH}}{\text{L soln}} = 1.67 \text{ M NaOH}
 \end{aligned}$$

As you can see, both methods give exactly the same result. Choose whichever method is most comfortable for you. Just remember that ultimately your units must be mol/L (= M).

Practice Problems

- What is the molarity of a solution that contains 1.724 moles of H_2SO_4 in 2.50 L of solution?
- What is the molarity of a solution prepared by dissolving 25.0 g of HCl (g) in enough water to make 150.0 mL of solution?