Online Laboratory calculus with automatic/instant Feedback (OLaF)

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Redaction:

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Mole introduction

For the majority of laboratory experiments, you have to make your own solutions from solid ingredients/chemicals. The required concentration is often given in mol/L. Mol is the unit of mole (similar to "g:" for grams or "L" for litre). It is the unit for a specific number of molecules. This specific number was based on the number of atoms present in 12 grams carbon-12 (C^{12}). The current definition (2019; www.nist.gov) is that "one mole contains exactly 6.022 140 76 × 10^{23} elementary entities". For kitchen salt, one "NaCl" molecule repesents the entity.

- ➔ 1 mol contains 6.022 140 76 x10^{23} particles or molecules (the Avogadro constant) of that substance.

Molarity is the amount of moles of a entity (for instance NaCl) present per litre of a solution. Molarity (a measure of concentration) is expressed by the symbol M which stands for mol/L (M = moles/litre).

To prepare a solution with a specific concentration, you need to know how many grams correspond to 1 mol of that specific substance. The amount of solid in grams per mol is known as the molecular weight (MW) and is often shown on packaging as the formula weight (FW).

- ➔ How do you determine the amount of grams needed of a certain substance to make the desired solution?

This can be calculated using the following formula: $M * MW * V = g$

M = desired molarity in mole per litre (mol/litre or mol * $litre^{-1}$)

MW = molecular mass given on the packaging in grams per mol (g/mol or g * mol^{-1})

V = the desired end volume of the solution

g = grams

The following parameters should be considered:

1. Determine the desired amount (V) of the solution (in litre)
2. Determine the desired molarity in mol per litre
3. Determine the molecular weight
4. Then calculate the amount of substance that should be weighed

Example: You need to make a sodium chloride (NaCl) solution with a molarity of 0.5 and a total volume of 3 Litres (MW = 58.44 g/mol). How many grams of NaCl are needed?

$M * MW * V = g$

0.5 * 58.44 * 3 = g

g = 87.66 grams

Concentrations expressed as percentage

The concentration of a solution can also be expressed as percentage (%) of one fluid (v) dissolved in another fluid (X% (v/v)) or the amount of millilitres dissolved per 100 ml mixed total solution. An example how to calculate the % concentration of a solution is given below. A similar calculation can be performed for 2 solids mixed together, this is called X%(m/m) for m= mass or X% (w/w) for w= weight, the amount of grams mixed per 100 gram mixed total solid. Finally, a solid can be dissolved in a fluid, which is indicated by X% (m/v) or X% (w/v) the amount of grams dissolved per 100 ml mixed total solution.

X%(v/v)	X ml dissolved fluid per 100 ml of solution
X%(m/m)	X gram solid per 100 gram mixed solid
X%(m/v)	X gram dissolved solid per 100 ml solution

Example: You have a 0.5M solution of sodium chloride (NaCl, MW = 58.44 g/mol). Calculate the X% of this solution**.**

The solution has a concentration of 0.5 mol/litre, and you have 100 ml (the X% is always expressed per 100ml). Accordingly, a 0.5M solution corresponds to 0.5 moles dissolved in 1 litre, or 0.05 moles per 100 ml.

0.5moles/10 = 0.05 moles.

Since 1 mole corresponds to 58.44 g, 0.05 moles correspond to

0.05 mol*58.44g/mol = 2.922 (rounded to 1 decimal) = 2.9 gram NaCl per 100ml = X% (m/v).

You have a 2.9% (w/v) solution. You would normally talk about a 2.9% solution.

Dilutions

To dilute concentrated solutions or solids, a diluent is needed.

➔ Diluent: the medium that is added to a certain concentrated solution or solid to dilute it. This can be distilled water, but also an organic diluent like ethanol, methanol or hexane.

In many protocols, a dilution factor is given as 1:X (pronounce 1 in X). 1 part of the concentrated solution is added to (X-1) parts of the diluent to achieve the desired dilution. The resulting solution has a concentration of 1/X times the concentration of the concentrated solution you started with (see examples in Table 1 and Figure 1). It is recommended to always write down the desired end concentrations in M (molarity) or in grams per litre to prevent any errors.

Table 1: Dilutions. Be careful! 1:1 (one in one, so no dilution!) is often mistakenly interpreted as 1:2 (one in two, that is one part in a total of two parts)! Similarly, the dilution factor 1:9 (one in nine) is often mistakenly interpreted as 1:10 (one in ten or a ten-fold dilution). The reason for these errors have to do with language and cooking. In cooking, we often refer to 1 ***to*** 1 (one part ***added to*** another part – which in science would be 1 ***dissolved in*** 2, or a two-fold dilution). When you encounter 1:1 or 1:9 in a protocol, check it carefully and ask what the intentions were here. Additionally, make a note of this in your lab journal, so you know afterwards what you did.

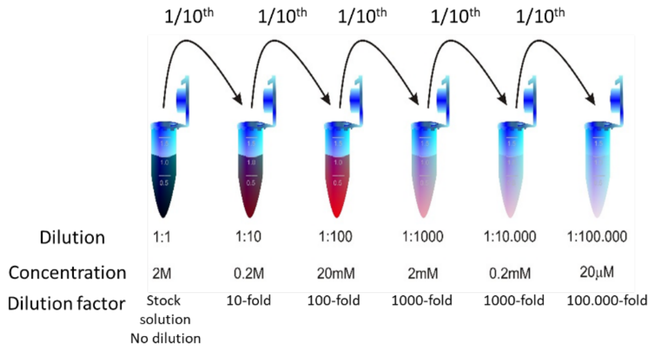


Figure 1: Dilution series**.** Every step represents a 10-fold dilution, or 1 part of the previous solution is diluted with 9 parts of the diluent (the following solution).

Dilution Factors			Concentration (example)
1:1 one part in a total of one		Undiluted	10M
1:2 (one in two)	= 2x diluted	1 part undiluted solution and 1 part diluent	5M
1:5 (one in five)	= 5x diluted	1 part undiluted solution and 4 parts diluent	2M
1:16 (one in sixteen)	= 16x diluted	1 part undiluted solution and 15 parts diluent	0.625M
1:100 (one in one hundred)	= 100x diluted	1 part undiluted solution and 99 parts diluent	0.1M

Example: You have to dilute 100mL of a 0.5M solution of sodium chloride (NaCl) 5-fold (or 5x) with distilled water. What will be the end volume and the molarity of the diluted solution?

100 mL (= 1 part) of the stock solution is added to 4 parts of distilled water --> total volume 500 mL (100 mL + 400 mL = one part in a total of 5 parts).

The concentration (molarity) of the diluted solution will be 0.1 mol/L. You diluted the original stock solution five-fold (0.5M/5 = 0.1M).

You can also calculate in a different way: you had 100 mL of a 0.5M solution, which contained 0.05 moles of NaCl. After the dilution, those 0.05 moles are contained in 0.5L. 0.05M/0.5L = 0.1 M/L

Conversions & Units

For each calculation, it is important that the correct units are used. You may have to express a concentration as molarity or as percentage, or you want to calculate an amount of a substance in a certain volume. You may start with grams/L but want to express it as micrograms per millilitre.

Table 2 shows an overview of the most common units in the laboratory and the associated factors. Always express your answer in the basic units (grams, moles, litre) unless stated or asked differently.

Table 2: Units overview

Factor		Weight		Volume		Mole	
			symbol		**symbol**		**symbol**
1.000	10^3	kilogram	kg	Cubic meter	m^3		
1	1	gram	g	Litre	l	mole	mol
0.1	10^{-1}			decilitre	dl		
0,001	10^{-3}	milligram	mg	millilitre	ml	Millimole	mmol
0.000,001	10^{-6}	microgram	µg	microlitre	µl	micromole	µmol
0.000,000,001	10^{-9}	nanogram	ng	nanolitre	nl	nanomole	nmol
0.000,000,000,001	10^{-12}	picogram	pg	picolitre	pl	picomole	pmol
0.000,000,000,000,001	10^{-15}	femtogram	fg	femtolitre	fl	femtomole	fmol

Example: You have 100 mg NaCl and want to dissolve this amount in 100 mL distilled water (MW = 58.44 g/mol), what is the molarity in mole per litre (mol/L or M)?

100 mg NaCl = 0.1 gram NaCl

0.1 : 58.44 = $1.71 * 10^{-3}$ mol NaCl

Volume = 100 mL = 0.1 L

You have $1.71 * 10^{-3}$ mol NaCl in 0.1 L. You want to express this in mol/L (10x 0.1L = 1.0 L)

$10 * 1.71 * 10^{-3} = 0.0171$ M = $1.71 * 10^{-2}$ M

OR if you prefer a crosstab:

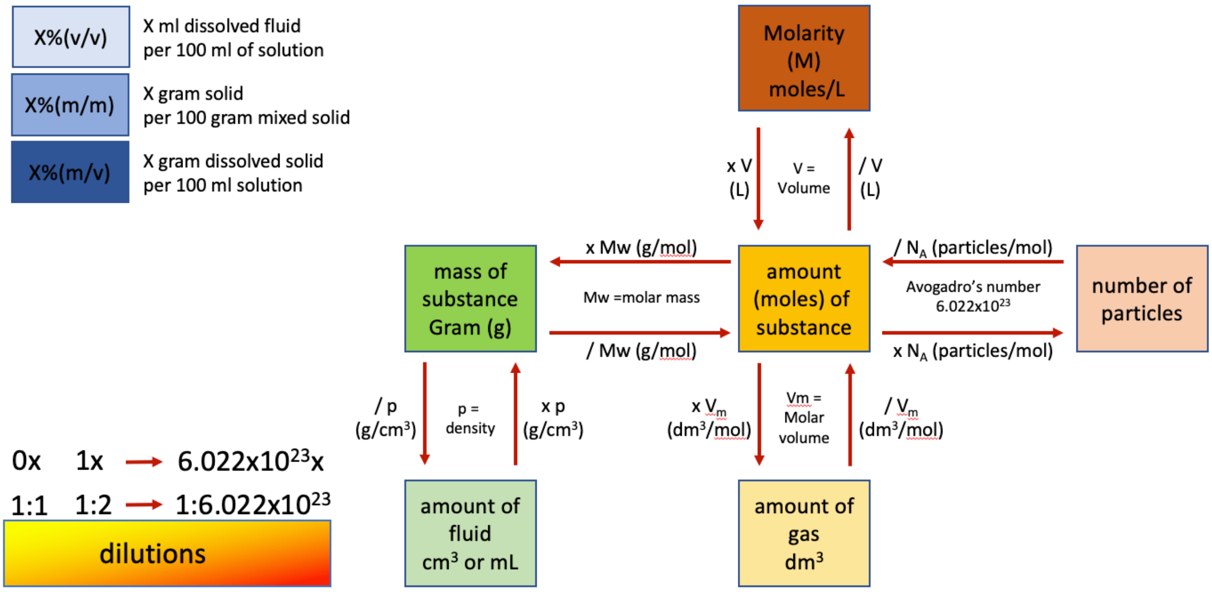
Mol	Litre
$1.71 * 10^{-3}$	0.1
x	1.0

$$x = \frac{1.71 \ * \ 10^{-3} * 1.0}{0.1} = 0.0171 \text{ M} \ = \ 1.71 \ * 10^{-2} \text{ M}$$

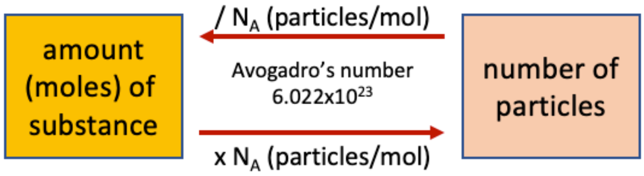
Chemical calculations

Often, you need several steps when performing chemical calculations to reach the desired answer. An overview of the most frequent steps is shown in Figure 2. The following paragraphs explain those separate steps. More complex questions that require combinations of several steps will be discussed later on.

Figure 2: Overview of chemical calculations



Number of Avogadro



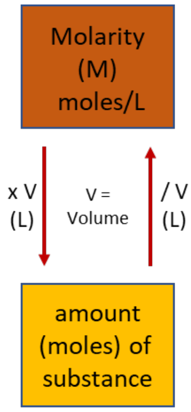
One mol is the unit for the amount of molecules of a certain substance. The current definition (2019; www.nist.gov) is that "one mole contains exactly 6.022 140 76 × 10^{23} elementary entities" (2019; www.nist.gov). This number is also known as the number of Avogadro, which can be used to convert the number of particles into the amount of substance into moles or the other way around, from mole to the amount of molecules/particles.

Example: How many particles/molecules are present in 5 mol NaCl?

5 * 6.022 140 76 x10^{23} = 3,0 x 10^{24} particles/molecules

Volume

Volume is an amount of fluid in litres or dm^3. The concentration of a substance is the number of moles per volume. If you know the volume, you can convert the amount of moles per litre (molarity) to the amount of the substance and the other way around.



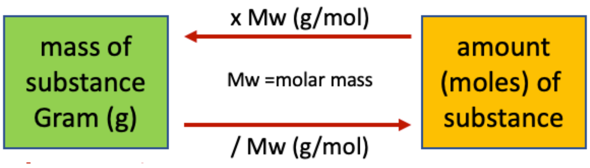
Example: You made a solution of 500 mL, which contains 5 moles of NaCl. Calculate the molarity (M) in mol per litre [mol/L]?

500 mL = 0.5 L

M = 5/ 0.5 = 10 mol/L

Molecular weight

Each molecule has its own specific weight, known as the molecular weight (MW), which is usually given on the packaging of the product or provided in the task/question (except when you are asked to calculate the molecular weight, of course). The amount of substance in grams per mol is known as the molecular weight, also known as molecular mass. With the MW, you can convert the amount in mol to the mass of the substance in grams or the other way around. For more information, see the subheading Mole introduction.

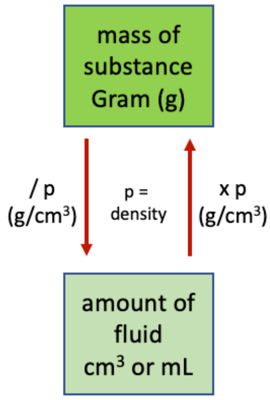


Example: You want to make a 1 M sodium chloride (NaCl) solution (MW = 58.44 g/mol) with a final volume of 1 litre. How many grams do have to dissolve?

You want 1 mol NaCl, so you need 58.44g in 1 litre. You use the MW for the conversion of grams to moles.

Density

Density is the ratio between the mass and the volume of a certain substance. This density determines which volume (in cm^3) a certain amount (g) of a specific substance occupies. The density allows you to convert the mass of a substance in gram into the amount of fluid in cm^3. The inverse calculation can, of course, also be performed. The density of water at 4°C at 1atm is roughly 1g/cm^3, accordingly, one ml or cm^3 of water weighs 1 g, or 1 litre almost exactly 1kg. Density (also called specific mass) is usually indicated by the symbol for the Greek letter *rho* = *ρ*, although *D* is also found. $\rho = m/V$ (with m for mass and V for volume).

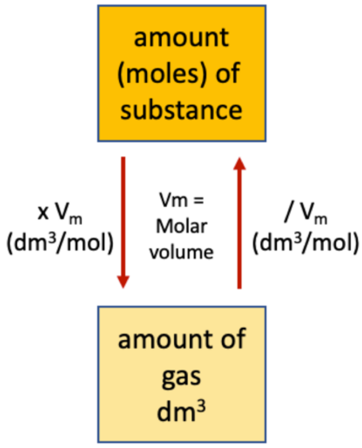


Example: Calculate the volume of 206 gram benzene in cm^3? (Density (D or *ρ*) = 0.72 g/cm^3)

206g/0.72 g/cm^3 = 268 cm^3

Molar volume

The molar volume is defined as the volume that contains exactly 1 mol of a substance at a given temperature and pressure and is indicated by V_m. V_m is mostly applied to gasses, however, it is actually equal to molar mass (M). The molar volume allows you to convert the amount of moles of a substance into the amount of gas in dm^3.



Example: At room temperature, oxygen has a molar volume of $2.45 * 10^2$ m^3/mol. 44 mol oxygen at room temperature occupy which volume in dm^3?

If you multiply the amount (in mol) with the molar volume, you get the volume in m^3. Then express this value in dm^3.

$44mol * 2.45 * 10^2\ m^3/mol = 10.8 * 10^2\ m^3 = 10.\ 8 * 10^5\ dm^3/mol$