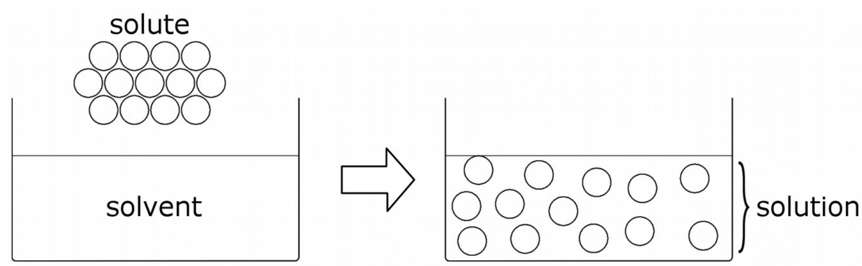
Solution composition

Definition of a solution

A solution is obtained when a solute is dissolved in a solvent (with "chemical" interactions). The solute can either be a solid, a liquid or a gas and the solute is either a liquid or a solid. (A gas-gas solution is not really a solution but rather a mixture)



The compound in smaller amount (number of particles) is the solute:
Ex: Identify the solvent when 60 g table sugar ($C_{12}H_{22}O_{11}$) is mixed with 40 g water:

$$60 \text{ g sugar} \times \frac{1 \text{ mole}}{342 \text{ g}} = 0.18 \text{ mol} \qquad 40 \text{ g water} \times \frac{1 \text{ mole}}{18 \text{ g}} = 2.2 \text{ mol}$$

mol(sugar) < mol(water), therefore, water is the solvent.

Homogeneous solution

The solvent and the solute are "chemically combined" or have strong intermolecular forces between them. An homogeneous solution has a unique boiling or melting point.

Heterogeneous mixture

Two or more phases are present even if they are not visible. The phases are physically mixed together but each phases retains its own chemical-physical properties. A heterogeneous mixture shows several boiling points and often, the solution is not transparent (milk, blood, etc.).

Butter = 35% water + milk fat, fatty acid, 120 different compounds,
Butter: T = 35 °C (fat melting), T = 110 °C (water boiling) T = 230 °C (fatty acids decomposition)

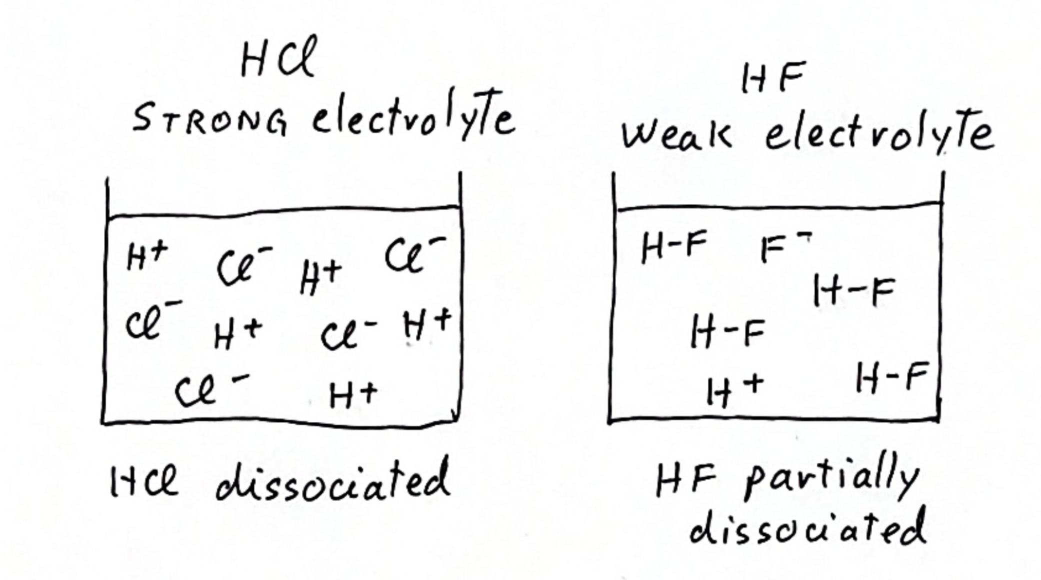
Type of solutions. Many types of solutions are possible:

		solvent	
		liquid	solid
solute	solid	Sugar or salt in water	Cu or Ag in gold
	liquid	Alcohol in water	Hg in aluminum
	gas	CO_2 in sea water	H_2 in carbon or platinum

Electrolyte

An electrolyte is a solute that produces ion when dissolved in a solvent.
(Arrhenius, Chemistry Nobel prize 1903)
A solution containing an electrolyte is called an electrolytic solution.
Since it contains ions, an electrolytic solution can conduct electricity (ion transport mechanism).

An electrolyte is called “strong” when it is completely dissociated in a solution.



$HCl(aq) \longrightarrow H^+(aq) + Cl^-(aq)$ — complete ionization

$HF(aq) \rightleftharpoons H^+(aq) + F^-(aq)$ — partial ionization

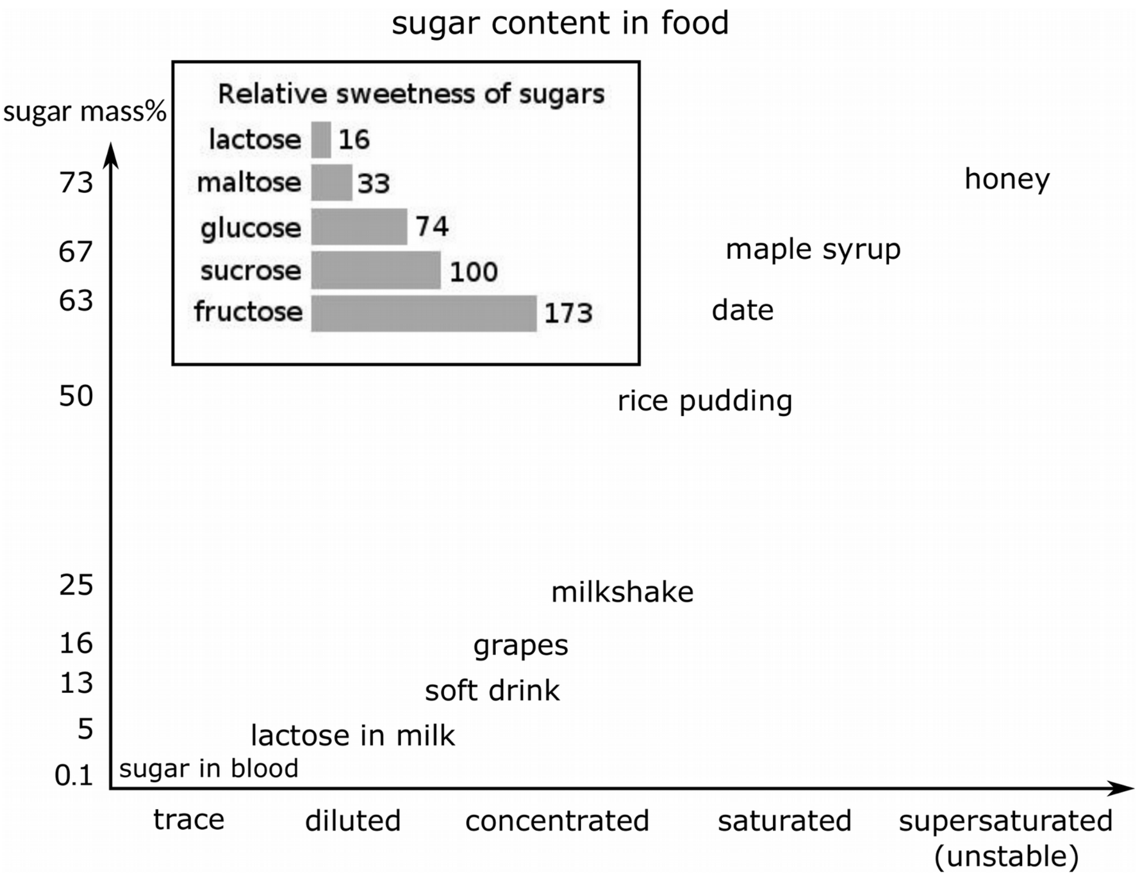
All the following solutes are water soluble (solvent).

Solute	Type of electrolyte	type	Conduct electricity
Soluble ionic compound KBr, NaCl,	Strong	Ionic	Yes
Strong base KOH, NaOH	Strong	Ionic (cation metal)	Yes
Strong acid HBr, $HClO_4$	Strong	Ionic covalent without metal	yes
Weak acid or base (partially dissociated) $HF \rightleftharpoons H^+(aq) + F^-(aq)$	Weak	Ionic covalent	Yes but poorly
Covalent molecule ethanol: C_2H_5OH sugar: $C_6H_{12}O_6$	Non electrolyte	Non ionic	No

Concentrations

The expressions "diluted" or "concentrated" are rarely used to express a concentration in chemistry since they are arbitrary values according to a specific condition.

For example, a white wine with a sugar concentration of 6 g/L is considered as low sugar alcohol while a blood sugar concentration higher than 1 g/L is considered as high.



Solubility

Solubility is the maximum amount (mass or mole) of a solute that can be dissolved in a solvent at a specific temperature

At 25°C: $NaCl$ = 39 g / 100 mL water
$AgCl$ = 0.0021 g / 100 mL water

The solubility is driven by the intermolecular forces (solute-solvent interactions, crystal lattice)

The SI symbol for concentration is "*c* "

The SI unit for molar concentration is mol/m^3 (IUPAC recommends mol/L)

Concentration is always a ratio: numerator = solute (smallest amount = dissolved)
denominator = solvent or solution (largest amount)

Concentration	Symbol	Units	use
mass%	%(w/w)	mass ratio: no unit	industries
part per million	ppm	(g solute / g solution) x 10^6	Analytical / environment
mole fraction	χ	molar ratio: no unit	physical chemistry
molarity	[ ] or *c*	mol/L or molar	laboratories
molality	m	mol/(kg solvent) or molal	physical chemistry
formality*	F	mol formula unit / L solution	fundamental research
normality*	N (discouraged)	equivalent / L	routine analysis

*Formality and normality are not used in chemistry NYB.

The use of the symbol "M" for molarity is discouraged since it is used in SI for mega or 10^6.

<u>Formality (F)</u>

Formality is similar to molarity but is specific to ionic compounds:

1 M NaCl(aq) does not exist in solution since only Na^+(aq) and Cl^-(aq) are present.

1 F NaCl(aq) makes sense. However, 1 M NaCl(aq) is still used in laboratories.

<u>Normality (N)</u>

Normality is based on the concentration of reactive species in a chemical reaction. Its interpretation changes depending on the chemical reaction present, therefore the use of normality (N) is discouraged by both NIST and IUPAC.

<u>For an acid base reaction:</u> 1 molar H_2SO_4 = 2 N H_2SO_4 (since 2 mol/L of H^+ are produced)

Normality is used for the concentration of standard acid solutions: HCl N/50 = 0.020 mol/L

<u>For an Oxidation-reduction reaction:</u>

$KMnO_4$, is a powerful oxidant. It consumes 5 electrons when it reacts, therefore:

1 molar $KMnO_4$, = 5 N since 5 moles of electrons/L are consumed by the $KMnO_4$ reactant:

$$KMnO_4 + 5e^- + 8H^+ \longrightarrow K^+ + Mn^{2+} + 4H_2O \quad \text{(reduction reaction)}$$

SI = Systeme International, IUPAC = International Union of Pure and Applied Chemistry,
NIST = National Institute of Standards and Technology (USA)

Specialized concentrations (NOT FOR NYB)

Concentration units must be practical. It changes according to the working environment.

- In a laboratory where temperature is controlled and glassware is designed to handle liquids with high precision, the molarity (mol/L) is the best unit of concentration to use.
- In industries that produce several tons of chemicals, the concentration used is the mass percentage.
- In environmental chemistry where trace contaminants are monitored, the unit of ppm is more appropriate.

In some fields, it is difficult to measure molarity accurately because the volume and density of the solution are unknown. This is the case when different temperatures are used.

In a thin-film lithium battery technology, the solvent is a polymer (plastic material) which can have a molar mass of several million g/mol. In this case, a convenient unit is the ratio of the number of moles of the polymeric repeating unit (solvent) to the mole of the dissolved electrolyte (solute):

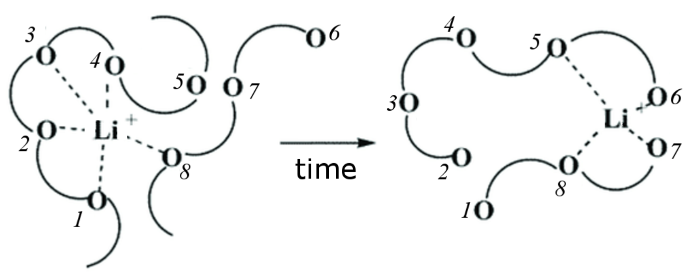
For example: polyethylene oxide + lithium salt = solid electrolyte solution.

The solute is an electrolyte: $LiClO_4$

The solvent is a solid polymer: polyethylene oxide: $-[CH_2-CH_2-O]_n-$ where "n" is large.

Transport of lithium ion in an amorphous solid PEO solution

concentration O/Li = 8/1



Schematic diagram of lithium ion conduction mechanism of PEO-based polymer electrolyte. [Reproduction with permission from Xu (2004), Copyright 2004, American Chemical Society].

Concentration = molar ratio O/Li

A concentration of : O/Li = 8 means ⇒ $-[CH_2-CH_2-O]_8-$ + $LiClO_4$

The mass ratio of this "solution" is 23.2% (w/w) of $LiClO_4$. However, it is more significant, in this field of research, to use a concentration of O/Li = 4, 8, 12 or 16, instead of using the mass percent.

Conversion between different concentrations

Concentration is an intensive property of the solution, so it does not change with the amount of solution used. To perform any conversion concentration calculation, you can use any mass or volume you want.

Any concentration conversion can be done as long as the molar masses of the components (solute and solvent) and the density of the solution are known. However, in some cases they are not always necessary.

From the mass, you can either know the amount (mole) or the volume by using any of the two conversion factor below.

Conversion factor:

mass ↔ (molar mass) ↔ mole

mass ↔ (density ρ) ↔ volume (at a specific temperature)

ρ is the symbol of density. It is often provided as:

- g/mL for a liquid
- g/cm^3 for a solid (1 mL = 1 cm^3)
- g/L for a gas

"*d*" is the symbol of the specific gravity.
It is the ratio of the density of a compound to that of water at the same temperature.

$$d_{20°C} = \frac{\rho(\text{compound})_{20°C}}{\rho(\text{water})_{20°C}} \quad \text{(no unit)}$$

PROBLEM: Concentration

Calculate the concentration (mol/L) of glucose in a cola can of 330. mL containing 35 g sugar (glucose, $C_6H_{12}O_6$, 180.2 g/mol)

$$c = \frac{mol}{L} \rightarrow \frac{mol = 35g \times \frac{1mol}{180.2g} = 0.194\ mol}{V = 330\ mL \times \frac{1L}{1000mL} = 0.330L} \rightarrow 0.59\ \frac{mol}{L}$$

Calculate the mass of KCl required to make 250.0 mL of a c = 0.750 mol/L solution

KCl = 74.55 g/mol

$$mol\ KCl = C \cdot V = 0.750\ \frac{mol}{L} \times 0.2500L = 0.1875\ mol$$

$$Mass\ KCl = 0.1875\ mol \times 74.55\ \frac{g}{mol} = 13.97 = 14.0\ g$$

What is the mass of H_2SO_4 (98.08 g/mol) present in a 5.00 g solution of c = 9.14 molar

The density of this solution is ρ = 1.498 g/mL

$$5.00\ g \times \frac{1\ mL}{1.498g} = 3.337\ mL$$

$$mol\ H_2SO_4 = 9.14\ \frac{mol}{L} \times 3.337\ mL \times \frac{1L}{1000mL} = 3.05 \times 10^{-2}\ mol$$

$$mass\ H_2SO_4 = 3.05 \times 10^{-2}\ mol \times \frac{98.08\ g}{mol} = 2.99g$$

PROBLEM: Concentration - conversion

Commercial aqueous nitric acid solution HNO_3(aq) is 70.%(w/w)

It has a solution density of: ρ(solution) = 1.42 g/mL

Calculate: The molarity, the molality and the mole fraction of HNO_3.

General informations:

HNO_3 = 63.01 g/mol

H_2O = 18.015 g/mol

Use any mass or volume of solution to start your calculations.

100. g HNO_3(aq)

- × 70.% = 70. g HNO_3 (mass solute)
- × 30. % = 30. g H_2O (mass solvent)
- $\times \dfrac{1.00\text{ mL}}{1.42\text{ g}}$ = 70.4 mL (volume solution)

Calculate the number of mole of each component in this sample:

Mole of solute: $70.\text{ g} \times \dfrac{\text{mol}}{63.01\text{ g}} = 1.11\text{ mol } HNO_3$

Mole of solvent: $30.\text{ g} \times \dfrac{\text{mol}}{18.015\text{ g}} = 1.67\text{ mol } H_2O$

Finally, find each concentration:

Molarity $= \dfrac{\text{mol}}{\text{L}} = \dfrac{1.11\text{ mol}}{70.4\text{ mL}} \times \dfrac{1000\text{ mL}}{1\text{ L}}$ = **16 mol/L** or molar

Molality $= \dfrac{\text{mol}}{\text{kg solvent}} = \dfrac{1.11\text{ mol}}{30.\text{g}} \times \dfrac{1000\text{ g}}{1\text{ kg}}$ = **37 mol/kg** or molal

Mole fraction $= \dfrac{\text{mol solute}}{\text{mol solution}} = \dfrac{1.11\text{ mol}}{1.11\text{ mol} + 1.67\text{ mol}}$ = **0.40** no unit.

The precision of the final answer is limited by the lowest significant number used for the calculation. Here, it is the mass% of HNO_3 = 70.% with 2 significant figures.

Dilution

$$\text{Concentration } (c) = \frac{\text{mol of solute}}{\text{volume of solution}}$$

A dilution-concentration process occurs when a solvent is added or removed by evaporation from a solution. Regardless of the amount of water added, the number of moles of solute is constant:

$$\text{Concentration (mol/L)} \times \text{volume (L)} = \text{number of mole (mol)}$$
$$c\,V = n$$

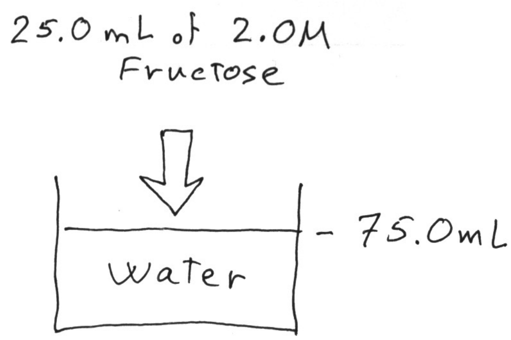
For an aqueous solution, where **only water is added or removed**, the number of mole of the solute remains constant then:

$$c_1\,V_1 = c_2\,V_2$$

V_1 is the initial volume of the solution while V_2 is the final volume of the solution after the addition or removal of the solvent.

a. Calculate the molarity of fructose in the final mixture:

25.0 mL of a 2.0 mol.L^{-1} solution of sucrose is added to 75.0 mL water



$$\text{molarity} = \frac{\text{mol of solute}}{\text{volume of solution}} = \frac{\text{mol}}{\text{L}}$$

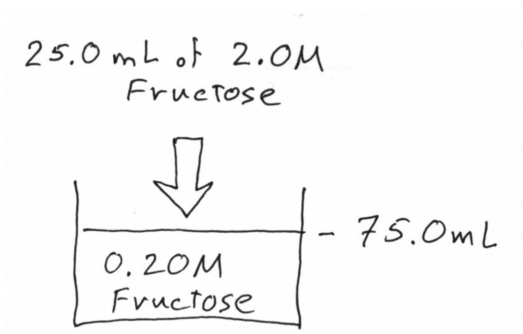
mole solute = 25.0 mL x 2.0 mol.L^{-1} = 50.$\underline{0}$ mmol

final volume solution = (25.0 + 75.0) mL = 100.0 mL

$$\text{concentration} = \frac{\text{mol}}{\text{L}} = \frac{50.\ \text{mmol}}{100.0\ \text{mL}}$$ = **0.50 mol.L^{-1}** (2 sig.fig.)

b. Calculate the molarity of fructose in the final mixture:

25.0 mL of a 2.0 mol.L^{-1} solution of sucrose is added to 75.0 mL of 2.0 mol.L^{-1} fructose



$$\text{molarity} = \frac{\text{mol of solute}}{\text{volume of solution}} = \frac{\text{mol}}{\text{L}}$$

final volume solution = (25.0 + 75.0) mL = 100.0 mL

Total mole fructose = (25.0 mL x 2.0 mol.L^{-1}) + (75.0 mL x 0.20 mol.L^{-1}) = 65.$\underline{0}$ mmol

$$\text{concentration} = \frac{\text{mol}}{\text{L}} = \frac{65.\ \text{mmol}}{100.0\ \text{mL}}$$ = **0.65 mol.L^{-1}**