Chemistry 201

Concentration conversions

NC State University

From mole fraction to molarity

The conversion from mole fraction to molarity can be solved analytically.

$$x_1 = \frac{n_1}{n_1 + n_2} = \frac{c_1}{c_1 + c_2}$$

Since $n_1 = c_1 V$ and $n_2 = c_2 V$ the V cancels out of each terms and we have

$$x_1(c_1 + c_2) = c_1$$

$$x_1 c_2 = c_1(1 - x_1)$$

From mole fraction to molarity

We can also write this as

$$x_1 c_2 = c_1 x_2$$

$$c_2 = c_1 \frac{x_2}{x_1}$$

Dilute solutions

Note that for water as solvent (component 1) x_1~ 1 and the concentration of water is c_1 ~ 55.56 M so that the conversion for a dilute solute such as a gas is c_2 ~ 55.66 x_2 M.

$$c_2 = x_2(55.56\ M)$$

This is very simple and quite useful (where it is a good approximation).

From mole fraction to molarity

For more concentrated solutions it is a poor approximation to assume that c_1 = 55.56 M. This assumption is only operative if the solvent is essentially pure water, i.e. $x_2 < 0.01$. For solutions with a significant component of co-solvent we cannot assume that the molarity of water is equal to that of a pure water solvent.

In the general case, we must consider the contribution of the relative mass of each component, which includes the molar mass as a weighting factor. The mole fraction is:

$$x_1 = \frac{m_1/M_{m,1}}{m_1/M_{m,1} + m_2/M_{m,2}}$$

where we have written the masses of each component, m_1 and m_2, separately.

From mole fraction to molarity

In a general procedure it is useful to assume that we have 1 L of solution. Therefore, the total mass has the same numerical value as the density (if given in units of kg/L, which is also numerically equal to the value in g/cm^3).

$$m_1 + m_2 = m_{total} = \rho(1\ \mathrm{L})$$

If we solve for m_2 and eliminate it from the equation above, then we find the following formula conversion factor (see Appendix).

$$n_1 = \frac{x_1}{x_1 M_{m,1} + x_2 M_{m,2}} m_{total}$$

From mole fraction to molarity

An analogous equation holds for n_2.

$$n_2 = \frac{x_2}{x_1 M_{m,1} + x_2 M_{m,2}} m_{total}$$

The conversion factor for both of the conversions from mole fraction to number of moles is equal to the total mass divided by the mole fraction weighted molar mass.

$$\frac{m_{total}}{x_1 M_{m,1} + x_2 M_{m,2}}$$

Note that n_1 and n_2 are numerically equal to c_1 and c_2 since we have assumed 1 L of solution

From mole fraction to molarity

For 1 L of solution, we can express the molarities as follows:

$$c_{1,2} = \frac{\rho}{x_1 M_{m,1} + x_2 M_{m,2}} x_{1,2}$$

One just needs to express the density in units of grams/liter since the molar masses are in units of grams/mole.

From mole fraction to molality

The conversion from mole fraction to molality is similar.

$$x_1 = \frac{n_1}{n_1 + n_2} = \frac{\boldsymbol{m_1}}{\boldsymbol{m_1} + \boldsymbol{m_2}}$$

We can reason the same way as used for molarity to obtain

$$\frac{x_1}{x_2} = \frac{\boldsymbol{m_1}}{\boldsymbol{m_2}}$$

Therefore,

$$\boldsymbol{m_2} = \boldsymbol{m_1}\frac{x_2}{1 - x_2}$$

This is rigorously true since the definition of molality is per kg of solvent.

From molality to molarity

One can convert from molality to molarity using the density as follows:

$$c_2 = \boldsymbol{m_2} \rho_1$$

For dilute solutions converting from molarity to molality involves the density of the solvent. We assume, in this case, that the solvent is the majority component and therefore, the volume of the solution (needed for molarity) is the same as the volume of the solvent.

$$\boldsymbol{m_2} = \frac{c_2}{\rho_1}$$

From molarity to molality

The method for converting from molarity is to assume 1 L of solution. If we assume 1 L of solution we can use the density to calculate the total mass,

$$m_{total} = \rho(1\ L)$$

The mass of the solvent is

$$m_1 = m_{total} - n_2 M_{m,2}$$

Once we know the mass of the solvent we can scale the molarity to calculate the molality.

$$\mathbf{m_2} = \frac{c_2(1\ L)}{m_1}$$

From molarity to mole fraction

For the conversion from molarity to mole fraction we will also assume 1 L of solution. As above we can obtain the total mass and therefore the mass of solvent, m_1. The number of moles of solvent is:

$$n_1 = \frac{m_1}{M_{m,1}}$$

We have n_2 from the assumption of 1 L of solution.

$$n_2 = c_2(1\ \mathrm{L})$$

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$$x_1 = \frac{n_1}{n_1 + n_2} \qquad x_2 = \frac{n_2}{n_1 + n_2}$$

From molality to mole fraction

For the conversion from molality to mole fraction we will also assume 1 kg of solvent. The number of moles of solvent is:

$$n_1 = \frac{1000\ \text{g}}{M_{m,1}}$$

We have n_2 from the assumption of 1 kg of solvent.

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$$x_1 = \frac{n_1}{n_1 + n_2} \qquad x_2 = \frac{n_2}{n_1 + n_2}$$

From mass fraction to mole fraction

The mass fraction defined above in section 1.2 can be converted into mole fraction by recognizing first how to express the mole fraction in terms of mass.

$$x_2 = \frac{n_2}{n_1 + n_2} = \frac{m_2/M_{m,2}}{m_1/M_{m,1} + m_2/M_{m,2}}$$

Then we see that the masses m_1 and m_2 can be converted to mass fractions by dividing both numerator and denominator by $m_1 + m_2$.

$$x_2 = \frac{mf_2/M_{m,2}}{mf_1/M_{m,1} + mf_2/M_{m,2}}$$

From mass fraction to mole fraction

By the same logic as above we can convert moles in the numerator and denominator to mole fraction by dividing both top and bottom by $n_1 + n_2$.

$$mf_2 = \frac{x_2 M_{m,2}}{x_1 M_{m,1} + x_2 M_{m,2}}$$

Throughout these steps we should keep in mind that the mass and mole fraction have the following relationship (for a two-component mixture).

$$mf_1 = 1 - mf_2 \qquad x_1 = 1 - x_2$$