Statistical Molecular Thermodynamics

Christopher J. Cramer

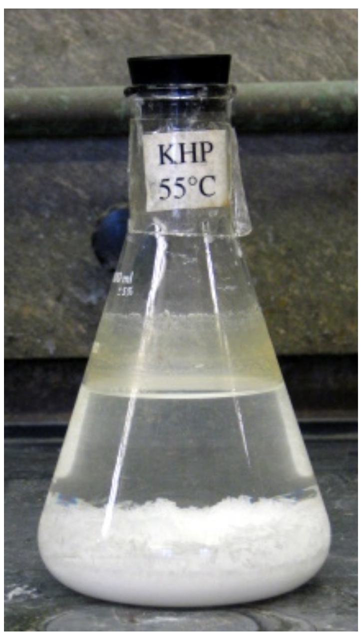
Video 11.1

Solutions with Solutes

Solutions with Solutes

So far, we've considered solutions of two components that range from pure 1 to pure 2

A more common situation is that we have one component, the "solvent" present to a much greater extent than the second component, the "solute"



←

In this solution, at equilibrium, the chemical potential of the *dissolved* *solid (the "solute") must be equal to the chemical potential of the* *pure* *solid. Solubility is thus* controlled *by the chemical potential — a topic of great economic importance to the pharmaceutical industry, for instance (as it affects the bioavailability of drugs).*

Convenient Units of Concentration

In the case where a solute has a limited solubility in a solvent, mole fraction is not a particularly useful variable to describe the solution, as the limiting mole fraction of the solute may be very near zero

It is generally more convenient to refer to concentrations of solutes in solution using mola<u>l</u>ity *or* mola<u>r</u>ity *scales*

These different choices for describing the relative proportions of solvent and solute are part of the "standard state" and must be monitored carefully when actual numeric data are being handled!

mole fraction *vs* molality *vs* molarity

Molality and Molarity

Definitions

<u>mole fraction</u>	<u>molality</u>	<u>molarity</u>
$x_2 = \dfrac{n_2}{n_1 + n_2}$	$m = \dfrac{n_2}{1\text{ kg solvent}}$	$c = \dfrac{n_2}{1\text{ L solution}}$
$0 \le x_2 \le 1$	$0 \le m \le \infty$	$0 \le c \le \infty$
unitless	mol kg^{-1}$_{solvent}$	mol L^{-1}$_{solution}$

$$x_2 = \frac{m}{\dfrac{1000\text{ g kg}^{-1}}{M_1\text{ g mol}^{-1}} + m}$$

M_1 is molecular weight
of the solvent
g mol^{-1}

$$c = \frac{\left(1000\text{ mL L}^{-1}\right)m\rho}{1000\text{ g kg}^{-1} + mM_2}$$

ρ is density
of the *solution*
g mL^{-1}

Self-assessment

mole fraction	molality	molarity
$x_2 = \dfrac{n_2}{n_1 + n_2}$	$m = \dfrac{n_2}{1\text{ kg solvent}}$	$c = \dfrac{n_2}{1\text{ L solution}}$
$0 \le x_2 \le 1$	$0 \le m \le \infty$	$0 \le c \le \infty$
unitless	mol kg^{-1}$_{solvent}$	mol L^{-1}$_{solution}$

$$x_2 = \frac{m}{\dfrac{1000\text{ g kg}^{-1}}{M_1\text{ g mol}^{-1}} + m}$$

M_1 is molecular weight of the solvent g mol^{-1}

$$c = \frac{\left(1000\text{ mL L}^{-1}\right) m\rho}{1000\text{ g kg}^{-1} + mM_2}$$

ρ is density of the *solution* g mL^{-1}

You mix 838.6 g sucrose with 471.7 mL water to get 1 L solution at 1 bar and 298 K; what is the mole fraction, molality, and molarity of the sucrose solution?

Self-assessment Explained

mole fraction

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

$$0 \le x_2 \le 1$$

unitless

molality

$$m = \frac{n_2}{1\text{ kg solvent}}$$

$$0 \le m \le \infty$$

mol kg^{-1}$_{solvent}$

molarity

$$c = \frac{n_2}{1\text{ L solution}}$$

$$0 \le c \le \infty$$

mol L^{-1}$_{solution}$

You mix 838.6 g sucrose with 471.7 mL water to get 1 L solution at 1 bar and 298 K; what is the mole fraction, molality, and molarity of the sucrose solution?

The molecular weight of sucrose is 342.3 g/mol, so 838.6 g is 2.450 mol (n_2). The molecular weight of water is 18.02 g/mol. At 298 K and 1 bar, water has a density of 0.997 g/mL, so 471.7 mL of water weighs 470.3 g and is thus 26.10 mol (n_1). The mole fraction is thus 2.450/(26.10+2.450) = 0.086, the molality is 2.450/0.4703 = 5.21 molal, and the molarity is trivial since we make exactly 1 L of solution, i.e., 2.45 molar. It may be a further useful exercise to verify to yourself that the conversion formulae on the prior slides that take one concentration measure to another do indeed work.

Next: Concentrations and Standard States