

Qualitative understanding of partition preferences

- Introduction
- ▼ Cavity model
 - ↓ ● **A simple model for bulk phase partitioning**
 - ↓ ● The cavity approach
 - ↓ ● The interaction energies
 - ↓ ● Polarity
 - ↓ ● Exercise
- ▶ Rules for partitioning
- The cavity model in quantitative terms
- ▶ Selftest
- ▶ Problems
- ▶ Intermolecular interactions in every day life
- FAQ

A simple model for bulk phase partitioning

The transfer of a molecule *i* from phase 2 to phase 1 requires that interactions between *i* and those molecules that make up phase 2 are given up while new interactions between *i* and molecules of phase 1 become possible. The more free energy, $\Delta_{12} G_i$, is released from a 2-phase-system by the transfer of one molecule *i* from phase 2 to phase 1 the higher will be the equilibrium concentration of *i* in phase 1. Or if we put it in more quantitative terms: there is a proportionality between the logarithm of the partition constant and the free energy of the partition process: (Note: per definition $\Delta_{12} G_i$ is negative if free energy is released.) (see [EP and the free energy of partitioning](#) in Chapter 2)

$$\ln K_{i\,12} \propto - \Delta_{12} G_i = - (G_{i1} - G_{i2})$$

In Chapter 2 we have argued that the preference of a solute molecule for a phase depends on its interactions in this phase. But this actually was an oversimplification. Partitioning into a phase always involves two steps and it is only the second of these two steps that depends on the interactions between the solute molecule and the surrounding phase molecules. This partitioning concept is called the cavity-approach.

