Qualitative understanding of partition preferences

- Introduction
- Cavity model
- A simple model for bulk phase partitioning
- The cavity approach .I.
- The interaction energies
- T. Polarity
- t. Exercise
- Rules for partitioning
- The cavity model in quantitative terms
- Selftest
- Problems
- Intermolecular interactions in every day life
- FAO

The interaction energies

For non-ionic organic compounds there are only two types of relevant interactions that we need to consider for a good qualitative understanding of partitioning: van der Waals interactions and H-bonds. The latter are more generally referred to as weak Lewisacid-base or electron-donor-acceptor interactions.

Note, in the literature one can find guite different categorizations of intermolecular interactions. Here we use the term "H-bonds" in a very wide sense because this allows a very simple approach to understanding partitioning. Others would use this term in a much narrower sense (i.e., restricted to compounds containing O or N) because this is more suitable on a quantum chemical level of understanding.

Fortunately, only little needs to be known about these intermolecular interactions for a good understanding of partitioning:

van der Waals interactions are always attractive and occur between any kind of molecules, even between water and alkanes. For a simple but convenient visualization of van der Waals forces all molecules may be thought of as being covered with some kind of glue. The strength of the attraction between molecules, particles or surfaces depends on both the stickiness of the glue and the contact area between interaction partners. The interesting thing about van der Waals interactions is that the 'stickiness of the glue' is rather similar for different organic compounds and even for water. Hence, a given molecule *i* exhibits similar van der Waals interactions in any organic phase and even in the water phase. As a consequence, van der Waals interactions cannot cause enormous differences in the partitioning constants of a given compound *i* in various condensed phases. However, the preference of most organic chemicals for the condensed organic phase as compared to the gas phase mostly results from van der Waals forces.

H-bond interactions are also always attractive but can only occur between a H-donor (i.e., e-acceptor) and a H-acceptor (i.e., e-donor). Hence, in contrast to van der Waals interactions,

sticks together when the complementary parts are in contact The energy of H-bond interactions depends on the number H-bonds that are formed as well as on their individual strength.



post-it.mov



velcro.mov

