Qualitative understanding of partition preferences

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Rules for partitioning of various compounds (1/5)

Above we have used the cavity concept to derive rules for the partitioning of a *given* compound *i* between a reference phase and *different* bulk phases. The same concept can also be applied to the relative partitioning of *different* compounds between *given* bulk phases. However, different features of the various interactions become important now. The relative partitioning of a *given* compound *i* between a reference phase and *different* bulk phases is hardly affected by van der Waals interactions because these interactions are similar for a given solute in various phases. When looking at the partitioning of *different* compounds with different size then differences in van der Waals interactions become important. But larger molecules not only exhibit larger van der Waals interactions they also possess a larger cavity energy. While the former favors partitioning from the gas phase into a condensed phase, the latter disfavors this process. Therefore it is important to know which of both counteracting processes wins. If the cavity energy only involves van der Waals interactions then it generally amounts to about half of the energy that a solute can gain from van der Waals interactions with the respective phase. And even in organic phases with a high number-density of H-bonds (e.g. ethanediol) does the total cavity energy (van der Waals component plus H-bond component) still not reach the energy that is gained by only the van der Waals interactions of the solute with the organic phase.

This has important consequences that can be formulated as rules:

Rule 5:

There is a linear trend between the logarithmic partition constants between air and apolar phases, In K

molecular size for any organic compound (see Figure 1).

Rule 6:

Organic molecules prefer to stay in any organic phase as compared to the gas phase because they always gain more energy in this phase (even if they only interact by van der Waals forces) than they will loose due to the cavity effect; i.e. $K_{i \text{ org.phase/air}}$ values are generally larger than 1.

