Equilibrium partitioning of organic compounds

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Equilibrium partitioning and the free energy of partitioning

All what we have said so far about the equilibrium partitioning of a chemical between various phases is captured by the following fundamental equation that relates the energy of interaction of *i* in two phases 1 and 2 to its partition constant, $K_{i\,12}$ at a given temperature:

$$\Delta_{12} G_i = -R\,T \ln K_{i\,12} \qquad (2)$$

where $\Delta_{12} G_i$ (J/mol) is the difference in the interaction energies per mol of *i* in the two phases 1 and 2. R is the universal gas constant (J/(mol K)) and T is the absolute temperature (K). This free energy is identical to the work that needs to be invested into the system to transfer one mol of *i* from phase 2 to phase 1.

We can evaluate equation (2) in order to see whether it is consistent with our previous understanding of partition equilibria: If the interaction energy is equal in both phases then the partition constant will be unity, i.e., the equilibrium concentrations of *i* in both phases 1 and 2 will be the same. If the interaction energy of molecule *i* in phase 1 is larger than the energy of i in phase 2 then energy is gained from the transfer of molecules *i* from phase 2 to phase 1 and $\Delta_{12} G_i$ is negative. In this case, $K_{i\,12}$ will be larger than unity which means that $c^*_{i\,1} > c^*_{i\,2}$. This shows that equation 1 is indeed in agreement with what we expect from the qualitative discussion on equilibrium concentrations.