

# Partitioning of Alkane and Alcohol Solutes between Water and (Dry or Wet) 1-Octanol

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## Abstract

Configurational-bias Monte Carlo simulations in the Gibbs ensemble using the OPLS (optimized potentials for liquid simulations) force field were performed to study the partitioning of normal alkane and primary alcohol solutes between water, neat or water-saturated 1-octanol, and helium vapor phases. Precise values of the Gibbs free energy of transfer were calculated directly from the ratio of the solute number densities in the two coexisting phases. It is observed that the OPLS force field yields Gibbs free energies of transfer that are in qualitative, albeit not quantitative agreement with experimental results. Comparison of the partitioning between a helium vapor and dry or wet 1-octanol phases established that water saturation affects mostly the partitioning of polar solutes, while differences for alkane partitioning were found to be negligible. In addition, the analysis of radial distribution functions of alcohol solutes in wet 1-octanol shows preferential partitioning into water-rich regions of the microheterogeneous solvent mixture.