Partition coefficients and possible solubilization sites of phenylalkanols in zwitterionic micelles

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We have measured limiting interdiffusion coefficients of phenylalkanols (benzyl alcohol, 2-phenylethanol, 3-phenyl-1-propanol, 4-phenyl-1-butanol, and 5-phenyl-1-pentanol) in water and aqueous micellar solutions of tetradecyltrimethylammonium bromide and obtained partition coefficients [1]. We have also made the measurements in solutions of dodecyl- and hexadecyltrimethylammonium bromide. In this study, we extended the measurements using zwitterionic surfactants, N-dodecyl-, N-tetradecyl-, and N-hexadecyl-N,N-dimethyl-3-aminio-1-propane sulfonates (C₁₂DAPS, C₁₄DAPS, C₁₆DAPS).

From the diffusion coefficients of phenylalkanols in water, $D_w$, and micellar solutions, $D$, as well as tracer diffusion coefficients of micelles, $D_m$, which were obtained by measuring the diffusion of pyrene solubilized in the micelles, we calculated the degree of association of phenylalkanols to micelles, $p$, from the relation

$$D = (1-p)D_w + pD_m \quad (1)$$

From the $p$ values we calculated partition coefficients of phenylalkanols between micellar pseudophase and bulk aqueous phase, $K_x = x_m/x_w$, where $x_m$ and $x_w$ are mole fractions of phenylalkanols in micellar pseudophase and bulk aqueous phase, respectively. Values for the standard free energy change for the solubilization, $\Delta G^0 = -RT\ln K_x$, were also calculated. For a given micelle, the $\Delta G^0$ values increase with increasing chain length of phenylalkanols; we compare the effect of the alkyl chain length with those for other systems. For a given phenylalkanol, $\Delta G^0$ values increase with increasing chain length of CₙDAPS. The increase is large from C₁₂DAPS to C₁₄DAPS, but not so large from C₁₄DAPS to C₁₆DAPS. The results are compared with those for alkyltrimethylammonium bromides, and possible solubilization sites are discussed.