

Solvation Energy Calculations of Homologous Trimethylammoniocarboxylates

Jennifer Lynn Kile

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Dr. Richard D. Gandour, Chairman

Dr. James M. Tanko

Dr. T. Daniel Crawford

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Abstract

Calculations of Solvation Energies of a Homologous Series of Betaines

Jennifer Lynn Kile

Calculating the solvation energies of surfactants is a way to predict the *cmc*. The solvation energies were determined for a homologous series of betaines, $(\text{CH}_3)_3\text{N}^+(\text{CH}_2)_n\text{COO}^-$ where $n = 1$ to 6. Their structure is composed of only the hydrophilic head group of a surfactant. The solvation energies were determined from both the gas phase energy and free energy of solution. Conformational analysis was performed on each molecule to locate the lowest energy structures and determine the Boltzmann population of each conformation for each molecule. The final solvation energies for each molecule are expectation values based on their energies and Boltzmann populations. The plotted solvation energies versus n form a parabolic curve that is similar to the literature *cmc* data where the betaine has a long hydrocarbon tail. However, the solvation energies peak at $n = 3$ and the *cmc* data peaks at $n = 4$. The dipole moments were also examined. The gas phase dipole moments were graphed and have a maximum at $n = 3$, similar to the solvation energy. The solution dipole moments have a linear graph, not comparable to the solvation energies. Therefore, the stability of the gas phase structures contributes more to the final solvation energy than the stability of the molecule in water.

The correlation between the plots of $\log \text{cmc}$ vs n and solvation energy vs n indicates that it is possible to computationally predict the *cmc* with this method. The hydrophobic contribution can be accounted for based on a known correlation between chain length and the *cmc*, and the hydrophilic contribution can be examined with this method. Therefore, it is possible to design a new surfactant molecule that has a *cmc* within the range of the biological activity to be sent for synthesis.

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