A Molecular Dynamics Study of the Free Energy of Micelle Formation for SDS in Water and its Size Distribution

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The free energy of micelle formation has been evaluated for spherical sodium dodecyl sulfate (SDS) in water by the thermodynamic integration method combined with a series of large-scale molecular dynamics calculations following the chemical species model. In particular, the free energy change, $\Delta\mu_{n1}^{0}$, with respect to the addition of one surfactant molecule to the spherical micelle of size n was obtained as a function of n. The free energy profile showed a minimum followed by a maximum, which corresponds to a peak in the size distribution. The calculated peak size n = 57 near its critical micelle concentration is in good agreement with the experimental averaged aggregation number, n = 55 – 75, of the SDS micelle. The distribution showed a rather sharp peak, indicating that the size is almost monodisperse. The size is likely to be insensitive to the total concentration of the surfactant.