MICHELLAR PHASE (L_1) TO HEXAGONAL COLUMNAR PHASE (H_1) TRANSITION IN SURFACTANTS AQUEUS SOLUTIONS: A MOLECULAR DYNAMICS SIMULATION STUDY

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ABSTRACT

Due to their amphiphilic nature, surfactant compounds are essential ingredients in various industrial products and applications, acting as detergents, wetting agents, emulsifiers, foaming agents, and dispersants.[1] In this study, using cetyltrimethylammonium chloride (CTAC) as a characteristic representative of the cationic surfactant family, we have developed a methodology based on Molecular Dynamics (MD) simulations, for predicting the phase behaviour of surfactants aqueous solution and in particular for estimating the concentration where the transition from the L_1 phase to the H_1 phase occurs for specific temperature (T) and pressure (P) conditions. A number of state points was excamined coverting the range of concentrations form 34 up to 70 wt% at T = 310 K and P = 1 atm. A detailed analysis of the orientational and positional order in the mesophases occurred in the simulation cells was performed,[2] and the results were compared against available experimenta data.[3,4] The proposed approach can be used for tuning the interactions parameters of the available atomistic force fields and coarse grained models of surfactant systems, based on their prediction on the properties of the demonstrated mesophases and their boundaries.

KEYWORDS: molecular modeling, surfactants, phase transition, CTAC

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