Molecular Dynamics Assessment of Concentration- and Head-Size-Dependent Effects on $C_{12}E_x$ Aggregation

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Since the dawn of the application of polymeric micelles as drug delivery systems in the late 1980s [1], numerous polymer self-assemblies have been extensively investigated, designated to deliver various substances including: low-molecular-weight anticancer drugs, contrast/imaging agents, proteins, plasmid DNA, antisense DNA, and more recently short interfering RNA (siRNA). Promising building blocks of drug delivery containers are deemed nonionic surfactants of poly(ethylene glycol) alkyl ethers, abbreviated as C_nE_x, where ***n*** refers to the number of carbon atoms in the hydrocarbon backbone of the tail and ***x*** – to the number of oxyethylene units in the hydrophilic head of the molecule.

The aim of the present study is to determine the head-size effect on the geometry transitions of $C_{12}E_x$ (***x***=3÷8) aggregates upon concentration increase. MARTINI [2] coarse-graining molecular dynamic simulations (NPT/293 K) of the self-assembly process of the listed surfactants in aqueous solution were carried out with PBC applied. Extending earlier estimates [3], aggregation numbers and aggregate shapes were defined and the concentrations at which certain shape transitions occurred were specified. The latter were quantified in terms of shape anisotropy supplemented by a detailed structural analysis of the micelles as a function of aggregation number.

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