Calorimetry and Molecular Dynamics Simulations for Surfactant-Cyclodextrin Inclusion Complexes

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Isothermal titration calorimetry and molecular dynamics simulations have been used to study the inclusion complexes between an anionic surfactant (sodium dodecyl sulfate, SDS) and two different cyclodextrins (α and β cyclodextrins). The stoichiometry of the complexes appears to change with cyclodextrin cavity size and also with temperature. To obtain the thermodynamic parameters characterizing the inclusion complexes, several thermodynamic models were used to fit the experimental calorimetric data. For α-cyclodextrin (αCD) complexes with 2:1 stoichiometry (αCD_2:SDS) were found to be stable, in equilibrium with the 1:1 species, while for β - cyclodextrin (βCD), the prevailing stoichiometry was 1:1 (βCD:SDS). To perform the molecular dynamics (MD) simulations different pre-formed SDS-CD complexes were considered in periodic boxes filled with simple point charged water molecules and were let to equilibrate for more than 10 ns. The simulations confirmed the stoichiometries found by the calorimetry data analysis. The analysis of the stable structures found in the MD simulations showed that H-bonding between two adjacent CDs is a key factor to produce stable CD_2:SDS complexes. The used combination of calorimetry and MD simulations can be the basis for a more general methodology to analyze complex self assembled structures.