EVALUATION OF SIMULATION BY BOUND WATER INVESTIGATION BASE ON DEUTERIUM NMR & DSC SPECTROSCOPY

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In order to evaluate computer simulation results on glycolipid bilayers and to determine an optimum configuration for the disaccharide head-group with respect to bilayer stability, we targeted to measure the bound water content for different alkyl glycosides and compare them with simulation results on hydrogen bonding between the surfactants and water. Several samples varying in D_2O concentration were prepared and D-NMR spectra were recorded. At usual temperatures, neither quadrupole splitting could be observed for lactosides nor for cellobiosides; instead only singlets were obtained. These results differ significantly from previous investigation on analogue maltosides, which exhibit powder patterns under similar condition. However, at high temperature, i.e. above 150 ºC, quadrupole splitting were detected. The quadrupole splitting increases with the D_2O concentration thus following the expected theory based trend. However, due to possible pressure development based on water vapor at these temperatures, the method is only applicable for samples containing low water contents. Unfortunately this range is insufficient for the investigation target. Besides this limitation, the quadrupole splitting exhibited an unexpected temperature response, i.e. increase with the temperature. Due to thermo induced disorder the quadrupole splitting, which reflects the overall orientation of O-D bonds, should decrease with rising temperature. The observed behavior can be explained if the splitting is not based on the D_2O probe, but reflects D-exchange of the OH groups of the sugar instead.

$$R\text{-}OH + D_2O = R\text{-}OD + HDO$$

As alternative methodology we applied DSC to determine bound water based on the melting enthalpy of water in the sample. Sample water can be grouped into three classes, i.e. isotropic free water, which encounters an environment similar to bulk water, oriented free water, which only interact with water but is affected by the orientation of water at the surfactant interface and the water which interacts directly with the surfactant. Only the former two types of water can freeze, thus the bound water can be determined by substituting the latter two from the total amount.

$$M_{bound\ eq} = M_{total\ eq} - M_{free\ eq}$$