

# About the solubilization of chiral guest molecules and the mechanism of the chiral induction in lyotropic liquid crystalline guest/host-systems

Summary of the doctoral thesis of Martin Pape

The presented thesis dealt with the mechanism of the chiral induction in discotic lyotropic nematic liquid crystals. The main parts are about the determination of the locus of chiral dopants with CD- and NMR-spectroscopy and the investigation of the dependence of the helical twisting power (HTP) of the chiral-nematic phase from molecular properties and of the intra- and intermicellar interactions from the temperature dependence of the pitch and the HTPs.

- Investigations with CD-spectroscopy show that the solubilization and the locii of  $\alpha$ -Hydroxycarboxylic acids and the Binaphthalene derivate BNDHP are independent of temperature and their concentration in the micellar solutions. In the N,N-Dialkyl-N,N-dimethylammoniumbromides the dopant molecules are solubilized nearly complete in the micelles, whereas in the perfluorinated alkanoates they penetrate the micelles less deep.
- The analysis of the CD signals leads to the conclusion that within the homologous series of the  $\alpha$ -Hydroxycarboxylic acids Phenylacticacid (PLA) shows a specific behaviour.
- The locii of chiral guest molecules have also been detected by the use of NMR-spectroscopy. The results of both spectroscopic methods show no contradictions.
- The HTPs in a group of hostphases depend on the chainlength and the size of the headgroup of the surfactant. The longer the alkylchain and the more voluminous the headgroup, the larger the HTP of a certain dopant in the hostphase. The transfer of the chirality of the dopants, which are solubilized in the core of the micelles could be explained with the modell of the intramicellar twist. The dopants with their chiral components in the outer of the micelles transport their chirality about interactions between the dopant molecules and the neighbored micelles.
- Propositions about the interactions between dopant and surfactant molecules could be derived by help of a molecularstatistical theory from the temperature dependence of the pitch. In the ammoniumbromides the dopants which are solubilized in the micelles show a dopant dependent behaviour. Dopants have been found that transport the chirality by a dispersive mechanism as well as dopants that prefer a sterical mechanism. However in the class of the perfluorinated alkanoates the trend of  $p(T)$  is independent of the used dopant. In all investigated cases a sterical mechanism could be detected. In case of the guest molecules with

the chiral parts of the molecules outside the micelles, it must be differed only between the two hostphase classes. In the ammoniumbromides the dispersive interactions overbalance the sterical ones and in the perfluorinated systems the inverse situation is found.

- The transfer of a model known from thermotropic liquid crystals to lyotropic systems shows that the temperature dependence of the perfluorinated systems is not influenced by the dopants but that it is a property of the hostphase.
- It is possible to define a geometrical parameter which describes the behaviour of different surfactant and hostphase classes respectively and which make it possible to estimate different properties of the investigated systems.

From this thesis many new insights could be extracted which lead to a better understanding of the chiral induction in lyotropic liquid crystalline systems. It is possible to determine the residence of the dopant molecules as well as to distinguish the interactions of guest and host molecules. It is still not possible to make predictions about the efficiency of a chiral molecule as dopant only by the knowledge of its chemical structure because of the multiplicity of the variables. The best examples for this proposition are the different effectivenesses of the sugar surfactants after the exchange of a single OH-group and the results of the  $\alpha$ -Hydroxycarboxylic acids.