Diffusion coefficients of perfluorinated *n*-alcohols in water and heavy water: experiment and computer simulation

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Fluorinated surfactants find nowadays many industrial applications due to their enhanced ability to lower surface tension in aqueous solutions [1]. As a result of their extensive use, emissions of fluorinated surfactants became frequent and, because of their persistent character, have been increasingly found in the environment [2]. Both the development of theoretical models to study the environmental fate of those pollutants and the design of unit operations (e.g. adsorption) used for their removal require the knowledge of some key properties such as the diffusion coefficients in water.

n-alcohols with perfluorinated carbon chains can be regarded as the most simple fluorinated surfactants, being suitable to be used as model substances that can make easier the molecular interpretation and the theoretical treatment of fluorinated surfactants in a systematic way. On the other hand, the smallest perfluorinated *n*-alcohols find applications in many fields, such as the pharmaceutical industry, polymer production and refrigerant technology as components of working fluids.

We have recently reported intra-diffusion coefficients of 2,2,2-trifluoroethanol in water for dilute solutions as a function of composition and temperature, obtained both experimentally (NMR spin-echo) and by computer simulation (molecular dynamics) [3]. The results obtained by molecular dynamics closely reproduce the experimental ones, which has encouraged us to attempt predicting the dynamic properties of aqueous solutions of the higher fluorinated alcohols and other fluorinated surfactants.

In this work, the intra-diffusion coefficients of 2,2,3,3,3-pentafluoropropan-1-ol, 2,2,3,3,4,4,4-heptafluorobutan-1-ol and 2,2,3,3,4,4,5,5,5-nonafluoropentan-1-ol in water and heavy water were measured experimentally by NMR spin-echo technique and compared with results obtained from computer simulation (molecular dynamics).

The comparison that can be done between experimental and simulation results is used to test the theoretical models for this chemical family of substances and enriches the molecular interpretation of the results, which can be useful to anticipate trends for more complex fluorinated surfactants.

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