

1. ABSTRACT

Initially, it was thought that lack of miscibility only occurred for liquids with significantly different properties. As a result, research on the phenomenon of microheterogeneity focused mainly on mixtures in which water was one of the components. In 2009, it was reported that the phenomenon of microheterogeneity was observed in a mixture of methanol and ethanol, i.e., liquids with similar physicochemical properties. The presence of separation at the molecular level for these alcohols may prove that this phenomenon is universal. The main goal of my doctoral thesis was to confirm the above hypothesis by searching for manifestations of microheterogeneity in a series of binary mixtures with different compositions and to determine the relationship between the structure of the mixture components and the structure of the liquid phase they create. Three types of mixtures were selected for testing: (1) where both components can form a hydrogen bond (water/alcohol, alcohol/alcohol), (2) only one of the components has this possibility (alcohol/hydrocarbon) and (3) none of the components forms hydrogen bonds (hydrocarbon/hydrocarbon). The tests were carried out over the entire range of mole fractions to determine the relationship between the mixture composition and the microscopic structure of the liquid phase.

Ingredients of the mixtures were selected in terms of different chain length and structure, and in the case of alcohols, also their order. As a basic research tool, we used vibrational spectroscopy (MIR and NIR), which allows obtaining information about the structure and intermolecular interactions occurring in the studied systems. The analysis of phenomena occurring at the molecular level was supported by the use of advanced computational tools, such as two-dimensional correlation analysis (2DCOS) and chemometric methods (PCA, EFA, MCR-ALS). These techniques allow for a detailed analysis of even small changes occurring in the studied systems, while using relatively large amounts of data generated by spectroscopic measurements. Additionally, theoretical calculations (DFT) of the structure of selected complexes were also performed in order to better understand the phenomenon of microheterogeneity in the tested mixtures. Combining the results of experimental research with the results of theoretical calculations made it possible to obtain a more complete characterization of the studied systems and contributed to a better understanding of the nature of elementary physicochemical phenomena occurring in the liquid phase.