Microheterogeneity in binary mixtures of aliphatic alcohols and alkanes : ATR-IR/NIR spectroscopic and chemometric studies.

Autorzy

Władysław Wrzeszcz

Paweł Tomza

Michał Kwaśniewicz

Sylwester Mazurek

Mirosław A. Czarnecki

Rok wydania

2016

Czasopismo

RSC Advances

Numer woluminu

6

Strony

94294-94300

DOI

10.1039/C6RA18692K

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Aliphatic alcohols form homogeneous mixtures with alkanes of similar size and structure, however at a molecular level one can expect the presence of both the homo and heteroclusters leading to the local heterogeneity. Recently, we observed this phenomenon in the binary mixtures of methanol with aliphatic alcohols [*RSC Adv.*, 2016, **6**, 37195]. This paper provides new and comprehensive information on the structure of alcohol/alkane mixtures at a molecular level. Besides, we studied the relationship between the chain structure and the deviation from the ideal mixture. A particular attention was paid for the difference between the linear and cyclic alcohols and alkanes. For studies we selected two alcohols: 1-hexanol, cyclohexanol, and two alkanes: *n*-hexane, cyclohexane. By combining these two pairs of compounds, we obtained four different alcohol/alkane mixtures. The inhomogeneity distribution of molecules in these mixtures and deviation from the ideality was characterized by ATR-IR/NIR excess absorption spectra and chemometric methods. Obtained results allow us to conclude that the separation at a molecular level and the extent of deviation from the ideality depends on the degree of association of the alcohol and the similarity of alkyl parts. As 1-hexanol is more associated than cyclohexanol, 1-hexanol/*n*-hexane mixture is the closest to the ideal mixture. In contrast, cyclohexanol/*n*-hexane is the most non-ideal mixture since in this case the smaller degree of self-association of cyclohexanol is coupled with different structure of alcohol and alkane chains.

Adres publiczny

http://dx.doi.org/10.1039/C6RA18692K

Strona internetowa wydawcy

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