

The effect of chain length on mid-infrared and near-infrared spectra of aliphatic 1-alcohols.

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Streszczenie

Effect of the chain length on mid-infrared (MIR) and near-infrared (NIR) spectra of aliphatic 1-alcohols from methanol to 1-decanol was examined in detail. Of particular interest were the spectra-structure correlations in the NIR region and the correlation between MIR and NIR spectra of 1-alcohols. An application of two-dimensional correlation analysis (2D-COS) and chemometric methods provided comprehensive information on spectral changes in the data set. Principal component analysis (PCA) and cluster analysis evidenced that the spectra of methanol, ethanol, and 1-propanol are noticeably different from the spectra of higher 1-alcohols. The similarity between the spectra increases with an increase in the chain length. Hence, the most similar are the spectra of 1-nonanol and 1-decanol. Two-dimensional hetero-correlation analysis is very helpful for identification of the origin of bands and may guide selection of the best spectral ranges for the chemometric analysis. As shown, normalization of the spectra pronounces the intensity changes in various spectral regions and provides information not accessible from the raw data. The spectra of alcohols cannot be represented as a sum of the CH₃, CH₂, and OH group spectra since the OH group is involved in the hydrogen bonding. As a result, the spectral changes of this group are nonlinear and its spectral profile cannot be properly resolved. Finally, this work provides a lot of evidence that the degree of self-association of 1-alcohols decreases with the increase in chain length because of the growing meaning of the hydrophobic interactions. For butyl alcohol and higher 1-alcohols the hydrophobic interactions are more important than the OH OH interactions. Therefore, methanol, ethanol, and 1-propanol have unlimited miscibility with water, whereas 1-butanol and higher 1-alcohols have limited miscibility with water.

Słowa kluczowe

atom, near-infrared spectroscopy, mid-infrared spectroscopy, spectra-structure correlations, molecule, chemometrics methods, principal component analysis, cluster analysis, MCR-ALS

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