

Molecular structure and hydrogen bonding in liquid cyclohexanol and cyclohexanol/water mixtures studied by FT-NIR spectroscopy and DFT calculations.

Autorzy

Mirosław A. Czarnecki

Andrzej S. Muszyński

Helena Troczyńska

Rok wydania

2010

Czasopismo

Journal of Molecular
Structure

Numer woluminu

974

Strony

60-67

DOI

10.1016/j.molstruc.2009.12.012

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The molecular structure and hydrogen bonding in liquid cyclohexanol and cyclohexanol/water mixtures has been examined by Fourier-transform near-infrared (FT-NIR) spectroscopy. FT-NIR spectra of pure cyclohexanol and binary mixtures with water at selected water mole fractions (x_w) from 30 to 80 °C and the spectra of the mixtures from $x_w = 0-0.4$ at 30 °C were measured. Besides, FT-IR and FT-NIR spectra of cyclohexanol in CCl_4 and cyclohexane solutions were recorded. The experimental spectra were analyzed by two-dimensional (2D) correlation approach and chemometrics methods. Interpretation of the spectra was guided by DFT calculations. It has been shown that small to moderate water content has a negligible effect on the structure of liquid cyclohexanol at constant temperature. Water molecules predominantly act as double donors to different species of cyclohexanol and this hydrogen bonding is stronger than that in bulk water. At lower water content appears a noticeable amount of singly bonded water molecules, however, population of this species in cyclohexanol is significantly smaller as compared with that in butyl alcohols. This results from much higher viscosity of cyclohexanol that stabilizes the cyclohexanol–water interactions. Increasing water content leads to creation of small clusters of water, where the water–water interaction is much weaker than that in bulk water. The temperature-induced breaking of smaller associates of cyclohexanol occurs easier in the presence of water, while an opposite effect was observed for the higher associates. The hydrophobic interactions in the cyclohexanol/water mixtures are of minor importance.

Słowa kluczowe

hydrogen bonding, Alcohols, Near infrared, two-dimensional correlation spectroscopy

Adres publiczny

<https://doi.org/10.1016/j.molstruc.2009.12.012>

Strona internetowa wydawcy

<http://www.elsevier.com>

Plik został wygenerowany dnia 2026-08-24 04:15:25

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/0M8JXmv>.