

Effect of temperature and water content on the structure of 1,2-propanediol and 1,3-propanediol: near-infrared spectroscopic study.

Autorzy

Krzysztof Z. Haufa

Mirosław A. Czarnecki

Rok wydania

2009

Czasopismo

Vibrational Spectroscopy

Numer woluminu

51

Strony

80-85

DOI

10.1016/j.vibspec.2008.10.013

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Effect of temperature and water content on the structure of 1,2-propanediol (12PD) and 1,3-propanediol (13PD) in the liquid phase has been studied by Fourier-transform near-infrared (FT-NIR) spectroscopy. In addition, the spectra of both diols in CCl_4 solutions at various concentrations were measured. The experimental spectra were analyzed by two-dimensional (2D) correlation approach and chemometric methods. The present results give no evidence that 12PD form the intramolecular hydrogen bonding. In contrast, significant amounts of 13PD molecules in diluted CCl_4 solution is involved in the intramolecular hydrogen bonding. At higher concentrations the intramolecular hydrogen bonds are broken and replaced by the intermolecular ones. The structure of pure liquid propanediols is determined by the intermolecular hydrogen bonding. Unlike for monohydroxyl alcohols, addition of water to propanediols leads to faster temperature-induced breaking of the hydrogen-bonded associates. However, variation of water content at constant temperature does not influence the structure of both diols. In this respect behavior of propanediols is similar to that of the monohydric alcohols. The molecules of water in the mixtures are hydrogen bonded to the diols and act as a double proton donor. This bonding appears to be stronger than that in bulk water.

Słowa kluczowe

Water/propanediols mixtures, Hydrogen bonds, Near-infrared spectroscopy, Two-dimensional correlation method

Adres publiczny

<https://doi.org/10.1016/j.vibspec.2008.10.013>

Strona internetowa wydawcy

<http://www.elsevier.com>

Plik został wygenerowany dnia 2026-10-13 14:10:29

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/2xd9yzl>.