Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Effect of temperature and concentration on the structure of *N*-methylacetamide-water complexes: near-infrared spectroscopic study.

Autorzy

Mirosław A. Czarnecki

Krzysztof Haufa

Rok wydania

2005

Czasopismo

Journal of Physical Chemistry A

Numer woluminu

109

Strony

1015-1021

DOI

10.1021/jp0471150

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Generalized two-dimensional (2D) FT-NIR correlation spectroscopy and chemometric methods have been used to study temperature-dependent spectral changes in pure *N*-methylacetamide (NMA) and NMA−water mixtures. We also examined the effect of varying water content on the structure of the mixture. It has been found that the extent of self-association of NMA in CCl_4 is very high; the association occurs even at concentration of 0.001 M. In the pure liquid NMA, the population of the monomers is negligible and the structure is dominated by the linear associates. An increase in temperature reduces the number of hydrogen bonds, but in contrast to alcohols their strength remains nearly the same. This reflects a difference in the mechanism of thermal breaking of the associates of NMA and alcohols. The present results reveal that the interaction between NMA and water in the NMA-rich region (X_{H2O} < 0.1) does not have a significant effect on the intrinsic structure of NMA. The structure of NMA is dominant, and the molecules of water do not form separate clusters but are dispersed and incorporated into the structure of NMA. We did not observe the presence of the free OH groups in the mixture. This led to the suggestion that each molecule of water forms two hydrogen bonds to two different molecules of NMA. An analysis of the asynchronous spectra reveals that most of the peaks observed in the asynchronous spectra, constructed from the temperature-dependent data, simply result from the frequency shift. This assumption is supported by the simulation studies.

Słowa kluczowe

Liquids, Mixtures, Molecules, Monomers, Noncovalent interactions

Adres publiczny

https://doi.org/10.1021/jp0471150

Strona internetowa wydawcy

https://www.acs.org/content/acs/en.html

Plik został wygenerowany dnia 2026-11-06 01:42:12

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/oipT-5Q.