

Near-infrared spectroscopic study of hydrogen bonding in chiral and racemic octan-2-ol.

Autorzy

Mirosław A. Czarnecki

Rok wydania

2003

Czasopismo

Journal of Physical Chemistry
A

Numer woluminu

107

Strony

1941-1944

DOI

10.1021/jp0270102

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The effect of temperature on self-association of (R)-(-)-octan-2-ol, (S)-(+)-octan-2-ol, and the racemic mixture in the pure liquid phase has been studied by two-dimensional (2D) Fourier transform near-infrared (FT-NIR) correlation spectroscopy. Both the conventional FT-NIR and 2D correlation spectra of pure enantiomers and the racemic mixture are identical to each other and do not reveal the chiral discrimination effect. The similarity of temperature relationships of population of the free OH groups for the optically active and racemic samples confirms the above conclusion. Of particular note is that the asynchronous spectra of all studied samples develop the peaks due to the free terminal OH groups in the open chain associates. This observation reveals a remarkable population of the linear species. The comparison of present results with previous studies on other isomers of octanol indicates that the degree of self-association decreases upon branching in the order octan-1-ol > octan-2-ol > octan-3-ol.

Słowa kluczowe

Alcohols, Mixtures, Molecular structure, Monomers,
Noncovalent interactions

Adres publiczny

<https://doi.org/10.1021/jp0270102>

Strona internetowa wydawcy

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