Dataset Paper

FTIR Spectra of n-Octanol in Liquid and Solid States

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The investigation of the temperature dependence of FTIR spectrum of n-octanol in the temperature range from -150°C to 50°C is presented. The observed changes in the registered spectra during gradual heating of the sample were analysed. The structure transformation at the phase transition from solid to liquid phase is detected.

1. Introduction

The alcohol molecules can form hydrogen bonds and arrange in different structures named clusters [1–4]. The work is devoted to the investigation of the temperature-dependent changes of cluster structure in n-octanol. Its chemical formula is $\text{CH}_3(\text{CH}_2)_7\text{OH}$. Among other fatty alcohols, n-octanol is widely used in industry, as a component of cosmetics and foods and as an industrial solvent. FTIR spectrum of liquid n-octanol at room temperature was presented earlier in [5]. In [6], the experimental FTIR spectra were compared with the results of quantum-chemical calculations for different cluster structures of n-octanol and an effect of cluster formation on the IR spectra was discussed.

In this paper, the registered FTIR spectra of n-octanol in the cycle of warming from the frozen state to the liquid state were investigated. The infrared spectroscopy was chosen as the experimental tool since any changes in cluster structure of the investigated object may be clearly detected by IR spectrum changes. Since the molecule of n-octanol is much longer than the molecules of simpler alcohols, such as methanol and ethanol, the identification of spectral bands is not so obvious [7–9].

2. Methodology

The presented spectra were registered in the laboratory of Fourier transform infrared absorption spectroscopy at the Physics Department of Vilnius University, Lithuania. All

spectra were recorded using Bruker's FTIR spectrometer VERTEX 70 equipped with LINKAM cryostat (model FTIR 600). The spectra were recorded in the spectral range from 750 to 4000 cm^{-1} and in the temperature range from -150 to 50°C . Liquid- N_2 -cooled mercury cadmium telluride (MCT) was used as a detector. Spectral resolution was 1 cm^{-1} and, in order to increase signal-to-noise ratio, each spectrum was taken as an average of 128 scans. Liquid n-octanol with purity > 99.9 from Fluka was used as received.

In Figures 1(a)–1(f), the registered FTIR spectra of n-octanol at different temperatures are presented.

The most intense spectral bands can be assigned as follows:

- (i) 998 cm^{-1} is assigned to in-phase stretch vibrations of C–O and C–C groups,
- (ii) 1059 cm^{-1} : stretch vibrations of C–O bond,
- (iii) 1479 cm^{-1} : scissoring vibrations of C–H bonds in CH_2 and CH_3 groups,
- (iv) 1465 cm^{-1} : antisymmetric (in relation to the plane C–C–O) bending vibration of C–H bonds in CH_3 group,
- (v) 1378 cm^{-1} : symmetric bending vibrations of C–H bonds in CH_3 .

Some spectral bands undergo some changes with the temperature increasing. The bands at 1159 cm^{-1} , 1202 cm^{-1} , and 1212 cm^{-1} observed in the frozen n-octanol disappear at

FIGURE 1: FTIR spectra of n-octanol at different temperatures: (a) 50°C, (b) -15°C, (c) -20°C, (d) -40°C, (e) -100°C, and (f) -150°C.

higher temperatures. Presumably, these bands are attributed to the rocking vibrations of CH_2 and CH_3 groups. The intensity of the spectral band at 998 cm^{-1} reduces during warming. The bands at 1037 cm^{-1} , 1054 cm^{-1} , and 1067 cm^{-1} merge into one intense band at 1056 cm^{-1} . The intensity of the spectral band at 1369 cm^{-1} decreases significantly with temperature increasing. The slight shift of the spectral band at 1462 cm^{-1} was registered at 50°C .

In the spectral interval $3000\text{--}4000\text{ cm}^{-1}$ for the frozen n-octanol, the following spectral bands were registered: 3167 cm^{-1} , 3228 cm^{-1} , 3287 cm^{-1} , 3314 cm^{-1} , 3402 cm^{-1} , 3440 cm^{-1} , and 3484 cm^{-1} . After heating, they are merged into one inhomogeneously broadened band centered at 3346 cm^{-1} . This band is attributable to the stretching vibrations of hydrogen-bonded hydroxyl groups.

It is widely known that the formation of large clusters in alcohols is accompanied by the decreasing of wavenumber of this band. For example, taking into account such shift for ethanol [8], it was concluded that, at low temperatures, this alcohol preferentially exists in the form of large clusters (consisting of six and more molecules). In the case of n-octanol, this shift is not so large and it can be concluded that, at low temperatures, the main contribution should be from trimers and tetramers, but a smaller fraction of pentamers and hexamers also should be present. Upon temperature increasing, the smaller clusters become absolutely dominant and, at room temperature, only ring tetramers and trimers should remain.

3. Dataset Description

The dataset associated with this Dataset Paper consists of 6 items which are described as follows.

Dataset Item 1 (Spectrum). FTIR spectrum of n-octanol at 50°C .

Dataset Item 2 (Spectrum). FTIR spectrum of n-octanol at -15°C .

Dataset Item 3 (Spectrum). FTIR spectrum of n-octanol at -20°C .

Dataset Item 4 (Spectrum). FTIR spectrum of n-octanol at -40°C .

Dataset Item 5 (Spectrum). FTIR spectrum of n-octanol at -100°C .

Dataset Item 6 (Spectrum). FTIR spectrum of n-octanol at -150°C .

4. Concluding Remarks

The registered FTIR spectrum of n-octanol changes with temperature increasing from -150°C to 50°C . The cluster structure of n-octanol is rebuilding upon transition from the

frozen to liquid state. At low temperature, one can observe the formation of both large and small clusters (trimers, tetramers, pentamers, and hexamers). With temperature increasing, the cluster structure is rebuilding and smaller clusters (trimers and tetramers) become dominant. The spectral band which is attributed to the stretch vibration of free hydroxyl group is not observed. This suggests that all clusters should have ring form.

Dataset Availability

The dataset associated with this Dataset Paper is dedicated to the public domain using the CC0 waiver and is available at <http://dx.doi.org/10.1155/2014/921308/dataset>.

Conflict of Interests

The authors declare that they have no conflict of interests regarding the publication of this paper.

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