

Studying the composition of alcohols using IR spectroscopy

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Abstract

In this article, we have determined the chemical composition of ethanol and 1-propanol using IR spectroscopy as a method. The absorption spectrum of ethanol is between the following wave numbers 3391cm^{-1} and 1056cm^{-1} . The absorption spectrum of 1-propanol is between the following wave numbers 3500cm^{-1} and 400cm^{-1} .

Keywords: Composition, ethanol, propanol, spectroscopy

Introduction

Infrared spectroscopy (IR spectroscopy) is a subset of spectroscopy that deals with the infrared region of the electromagnetic spectrum. It can be used to identify compounds or to investigate the composition of a sample.

The infrared spectrum of a sample is collected by passing a beam of infrared light through the sample. Examination of the transmitted light reveals how much energy is absorbed at each wavelength. This can be done using a Fourier transform instrument to measure all wavelengths simultaneously. From this, a transmission or absorbance spectrum can be generated that indicates at which IR wavelengths the sample absorbs. Analysis of these absorption properties reveals details about the molecular structure of the sample.

Infrared spectrometer, 4000 to 400cm^{-1} with main instrument bank a slightly narrower analysis range (from 4000 to approximately 650cm^{-1}) when using a totally attenuated reflector accessory and data) provides [1-5].

Thin coatings can be evaluated directly on a reflective substrate (reflectance absorption mode), and powder materials can be evaluated using the diffuse reflectance mode.

Almost any sample can be evaluated using the FTIR spectroscopy analysis method. Samples can be solid, liquid, or gaseous. Small samples can be analyzed in the instrument; larger samples can be analyzed using an external microscope accessory. The microscope can also be used to focus on a specific portion of a sample.

Solids and liquids are most commonly evaluated using FTIR spectroscopy. Solid materials can be thermosetting or thermoplastic materials, rubber materials, coatings, fibers, and virtually any manufactured product. Liquid samples include lubricants, solvents, contamination removed from a surface, and other liquids that need to be identified [6-18].

Material and Methods

Figure 1 shows the equipment necessary to determine the FTIR spectrum of alcohols.



Fig 1: Nicolet Avatar FTIR Spectrometer

Results and discussion

Alcohols have characteristic IR absorptions associated with both the O-H and the C-O stretching vibrations. When run as a thin liquid film, or "neat", the O-H stretch of alcohols appears in the region $3500\text{--}3200\text{cm}^{-1}$ and is a very intense, broad band. The C-O stretch shows up in the region 1260--

1050cm^{-1} .

- O-H stretch, hydrogen bonded $3500\text{--}3200\text{cm}^{-1}$

- C-O stretch $1260\text{--}1050\text{cm}^{-1}$ (s)

The spectrum of ethanol is shown below. Note the very broad, strong band of the O-H stretch (3391cm^{-1}) and the C-O stretches ($1102, 1055\text{cm}^{-1}$).

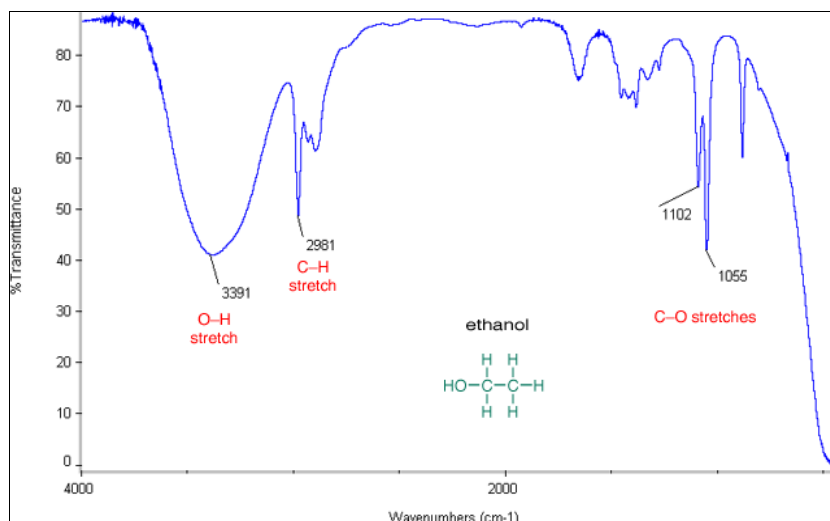


Fig 2: IR spectrum for ethanol

Table 1: Peak assignment in the FTIR spectrum of ethanol

Wave number, cm^{-1}	Functional grouping	Vibration mode
3391	O-H	stretch
2981	C-H	stretch
1102	C-O	stretches
1056	C-O	stretches

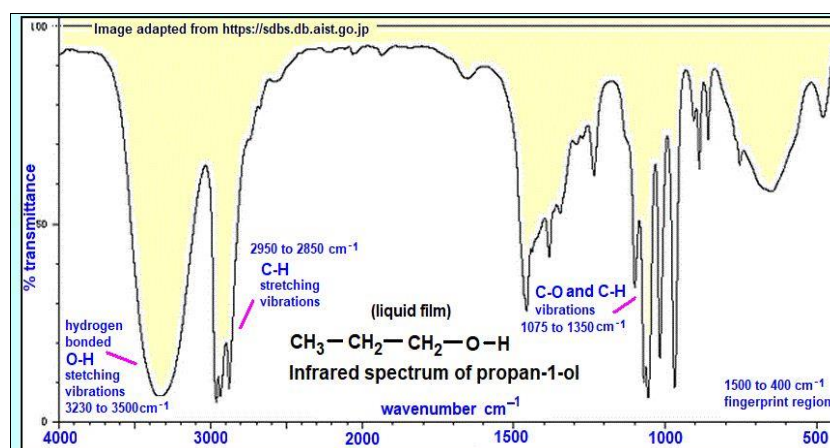


Fig 3: IR spectrum for 1-propanol

Spectra obtained from a liquid film of propan-1-ol. The right-hand part of the infrared spectrum of propan-1-ol, wavenumbers ~ 1500 to 400 cm^{-1} is considered the fingerprint region for the identification of propan-1-ol and most organic compounds. It is due to a unique set of complex overlapping vibrations of the atoms of the molecule of propan-1-ol. For propan-1-ol, the most characteristic absorption is the broad O-H stretching vibration band at wavenumbers ~ 3500 to 3200 cm^{-1} , the

breadth is caused by hydrogen bonding interactions, common to all hydrogen bonded molecules with a hydroxyl group e.g. alcohols and carboxylic acids. C-H stretching vibration absorption occurs $\sim 2900 \text{ cm}^{-1}$, wavenumbers common to any molecule with alkyl groups such as the propyl group in propan-1-ol.

There are wavenumber C-O and C-H vibration absorption bands ~ 1350 to 1070 cm^{-1} for propan-1-ol.

Table 2: Peak assignment in the FTIR spectrum of 1-propanol

Wave number, cm^{-1}	Functional grouping	Vibration mode
3230-3500	O-H	stretch
2950-2850	C-H	stretch
1350	C-O	stretches
1075	C-H	stretches

Conclusions

Ethanol and 1-propanol contain in IR only bands characteristic of functional groups: alcohols and alkanes.

Around 3200 - 3550 cm^{-1} , a broad, strong absorption band is often observed. This corresponds to the stretching vibration of the O-H bond in the alcohol group. The broadness is due

to hydrogen bonding. A sp^3 C-H stretch around $2850\text{--}2960\text{ cm}^{-1}$ will be present, corresponding to the C-H bonds in the alkyl group attached to the hydroxyl group. The C-O stretching vibration typically appears around $1000\text{--}1300\text{ cm}^{-1}$. This is a medium to strong band. Below 1500 cm^{-1} , you may observe various complex bands, which can help in identifying the unique structure of the alcohol.

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