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Study of the composition of aromatic hydrocarbons using IR spectroscopy

Ioana Stanciu*
Faculty of Chemistry, Department of Physical Chemistry, University of Bucharest, Bucharest, Romania

Abstract

In this article we have determined the chemical composition of toluene using IR spectroscopy as a method. The absorption spectrum is comprised between the following wave numbers 3099cm^{-1} and 738 cm^{-1}. -3050 cm^{-1}: Aromatic group C-H stretch - 3050 cm^{-1}, methyl group (–CH_3) C-H stretch - 2850-2960 cm^{-1}, aromatic group C=C stretches -1400-1600 cm^{-1}, aromatic group C-H out-of-plane bends -750-800 cm^{-1} and methyl group bending vibration -1370 cm^{-1}.

Keywords: Toluene, composition, hydrocarbon, spectroscopy

Introduction

Analysis by IR absorption spectrometry can be applied to gases, liquids or solids. Gases are introduced into special cells where the sample is introduced with the necessary precautions (rinsing, evacuation of the previous gas, vacuuming) or by dilution in air. Liquids can be studied as such or in the form of solutions. If they are too volatile, liquids can be analyzed by placing a drop between two perfectly polished discs made of NaCl crystals, which are subsequently pressed together and clamped in a frame before being introduced into the spectrometer. Solutions with concentrations between 0.05-10% are introduced into cells 0.1-1mm thick which are introduced as such into the IR spectrophotometer. Obviously the solvents must be anhydrous, pure and transparent in IR for the field of interest. The preferred solvents for dilutions are CCl_4, $CHCl_3$ and CS_2. Solids are analyzed either in solutions or as emulsions in paraffin oil. Emulsions in crystalline KBr can also be used at a dilution of 1% (1mg substance per 99mg KBr). The transparent pellet, obtained after grinding and pressing, is fixed in a suitable frame and inserted into the apparatus in front of the IR beam [1-9].

As mentioned, in recent years the Fourier transform IR analysis technique (FTIR) has been preferred, which results in changes in the vibrational energy of the molecule, and the absorbed energy is used to change the energy levels associated with them. It is a valuable tool for identifying organic compounds that have polar chemical bonds (such as OH, NH, CH, etc.) with good charge separation (strong dipoles). This technique uses a single beam of undispersed light.

In FTIR, the undispersed light beam is passed through the sample and the absorbances at all wavelengths are received at the detector simultaneously. To obtain absorption information for each wavelength, a computer mathematical manipulation (known as the "Fourier Transform") is performed on the obtained data. To perform this type of light interference calculations, a model is required for which the FTIR spectrophotometer contains two mirrors, one fixed and one movable with a beam splitter between them. Before scanning the sample, a reference is scanned or a blank scan is required [9-18].

Material and methods

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

Fig 1: Nicolet Avatar FTIR Spectrometer

Results and discussion

The =C–H stretch in aromatics (usually few bands) is observed at 3100-3000 cm^{-1}. Note that this is at slightly higher frequency than is the –C–H stretch in alkanes. This is a very useful tool for interpreting IR spectra: Only alkenes and aromatics show a C–H stretch slightly higher than 3000 cm^{-1}, alkenes typically single band at about 3080 cm^{-1}, aromatics few bands between 3100-3000 cm^{-1}. Compounds that do not have a C=C bond show C–H stretches only below 3000 cm^{-1}.

-2000-1665 cm^{-1} (few weak bands known as "overtones")
- 900-675 cm^{-1} (out-of-plane or "oop" bands)

Not only do these bands distinguish aromatics, but they can be useful if you want to determine the number and positions of substituents on the aromatic ring. The pattern of overtone bands in the region 2000-1665 cm^{-1} reflect the substitution pattern on the ring. The pattern of the oop C–H bending bands in the region 900-675 cm^{-1} are also characteristic of the aromatic substitution pattern.

Summary

- C–H stretch from 3100-3000 cm^{-1}, few bands
- overtones, weak, few bands, from 2000-1665 cm^{-1}
- C–C stretch (in-ring) from 1615-1590 cm^{-1}
- C–C stretch (in-ring) from 1500-1400 cm^{-1}
- C–H "oop" from 900-675 cm^{-1}

The spectrum of toluene is shown below. Note the =C–H stretches of aromatics (3099, 3068, 3032 cm^{-1}) and the –C–H stretches of the alkyl (methyl) group (2925 cm^{-1} is the only one marked). The characteristic overtones are seen from about 2000-1665 cm^{-1}. Also note the carbon-carbon stretches in the aromatic ring (1614, 1506, 1465 cm^{-1}), the in-plane C–H bending (1086, 1035 cm^{-1}), and the C–H oop (738 cm^{-1}).

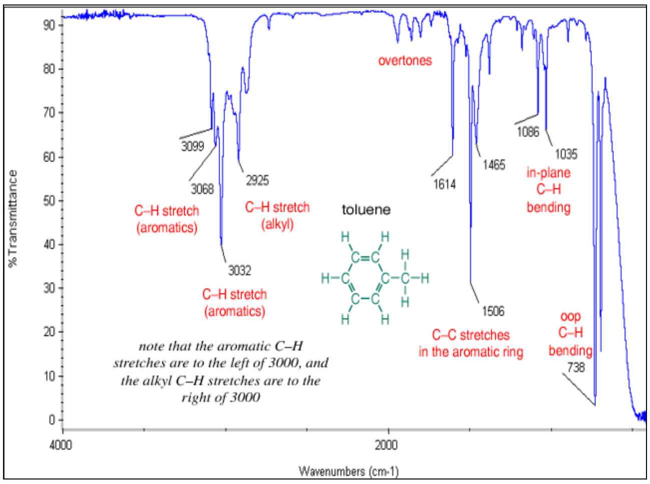

Fig 2: IR spectrum for toluene

Table 1: Peak assignment in the FTIR spectrum of toluene

Wave number, cm^{-1}	Functional grouping	Vibration mode
3099	C-H	stretch(aromatic)
3068	C-H	stretch(aromatic)
3032	C-H	stretch(aromatic)
2925	C-H	stretch(alkyl)
1614	C-C	stretches
1506	C-C	stretches
1465	C-C	stretches
1066	C-H	bending
1035	C-H	bending
738	C-H	bending

Conclusions

Toluene contains in IR only bands characteristic of functional groups: aromatic and methyl. Around 3050 cm^{-1}, a set of weak to medium intensity peaks appear, corresponding to the C-H stretching vibrations of the aromatic ring (benzene). Around 2850-2960 cm^{-1}, you will see C-H stretching vibrations from the methyl group ($-CH_3$) attached to the benzene ring. This is due to the methyl ($-CH_3$) group in toluene. Between 1400-1600 cm^{-1}, you'll find C=C stretching vibrations from the aromatic ring. This is a characteristic feature of aromatic compounds, usually appearing as two bands. Around 900-1100 cm^{-1}: You will observe some overtones and out-of-plane bending vibrations from the aromatic ring. These are often seen as multiple smaller peaks. Around 750-800 cm^{-1}: The out-of-plane C-H bending vibrations for the aromatic ring will appear as distinct peaks, typically indicating the substitution pattern of the benzene ring. Around 1370 cm^{-1}, you may observe a methyl bending vibration for the methyl group attached to the benzene ring. Below 1500 cm^{-1}, you will find a series of complex peaks representing the fingerprint region of the molecule. These are characteristic of the toluene structure.

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