National Journal of Advanced Research
www.thestudiesjournal.com
ISSN: 2455-216X
Received: 26-10-2025, Accepted: 25-11-2025, Published: 10-12-2025
Volume 11, Issue 2, 2025, Page No. 63-64

Study of the composition of nitriles 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 nitrotoluene and nitromethane using IR spectroscopy as a method. The absorption spectrum of nitrotoluene is between the following wave numbers 1537cm^{-1} and 1358 cm^{-1}. The absorption spectrum of nitromethane is between the following wave numbers 1573cm^{-1} and 1383cm^{-1}.

Keywords: Nitrotoluene, nitromethane, composition, spectroscopy

Introduction

The chemical bonds of molecules vibrate at different frequencies, depending on the elements that are bonded and the type of bond. For each bond, there are several specific frequencies at which they can vibrate. According to quantum mechanics, these frequencies correspond to the ground state (lower frequencies) and excited states (higher frequencies). One way to increase the frequency of a molecular vibration is to excite the bond by absorbing light energy. For any transition between two states, the energy of the light – determined by its wavelength – must be exactly equal to the energy difference between the two states (usually the ground state and the first excited state) [1-3]. The energy corresponding to the transitions between the molecular vibration states is generally between 1 and 10 kcal/mol and corresponds to the infrared portion of the electromagnetic spectrum [4-7].

Functional groups in molecules absorb infrared radiation in a specific range of wavenumbers, regardless of the structure of the rest of the molecule. Thus, a particular mode of motion of a chemical bond always occurs around a specific wavenumber. Correlating the wavenumber of the band with the chemical structure is used to identify the functional group of the sample [8-18]. The wavenumbers at which functional groups absorb are practically independent of temperature, pressure, the method of sampling, or changes in the structure of other parts of the molecule. Thus, the presence of specific functional groups in molecules can be revealed by these types of IR bands, called group wavenumbers.

In IR spectroscopy, the sample – subjected to infrared radiation – absorbs some of the radiation, while other parts pass through it or are transmitted. The resulting spectrum consists of the absorption and transmission of radiation and represents a true fingerprint of the analyzed substance, the absorption bands corresponding to the frequencies of vibrations of the bonds between the atoms of which it is composed, each substance being a unique combination of atoms [1, 3]. This means that IR spectroscopy can be used to identify chemical substances – for qualitative analysis. Since the size of the band is a direct indication of the amount of compound present, IR spectroscopy can also be used for quantitative analysis.

The first IR spectrometers, also called classical, are of the dispersive type, using a prism or a grid to separate the individual frequencies emitted by the source. The detector measures the amount of energy at each of the frequencies that pass through the sample. The result is a spectrum, in which the intensity is plotted as a function of frequency.

In the case of classical spectrometers, the spectral absorption of a sample is scanned, which makes the time to obtain the spectrum long. It is therefore necessary to use a method that measures all frequencies simultaneously and not individual frequencies. The solution consisted in using an interferometer, which measures all IR frequencies simultaneously. But in this case, the spectrum is not measured directly, but the interferogram. This is transformed into a spectrum by Fourier transformation, thus resulting in Fourier transform IR spectroscopy, FTIR [4].

Compared to conventional IR spectroscopy, FTIR has the following advantages [5]:

- the interferometer uses all wavelengths at the same time, reducing the observation time;
- the amount of radiation that passes is greater than for conventional monochromators;
- the accuracy of wavenumbers is better;
- the resolving power is greater.

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 N–O stretching vibrations in nitroalkanes occur near 1550 cm^{-1} (asymmetrical) and 1365 cm^{-1} (symmetrical), the band at 1550 cm^{-1} being the stronger of the two. Actually, both the bands are very strong in comparison to the bands of other functional groups.

If the nitro group is attached to an aromatic ring, the N–O stretching bands shift to down to slightly lower wavenumbers: 1550-1475 cm^{-1} and 1360-1290 cm^{-1}.

Summary:

- N–O asymmetric stretch from 1550-1475 cm^{-1}
- N–O symmetric stretch from 1360-1290 cm^{-1}
- See spectrum of *m*-nitrotoluene below. In nitrotoluene, the N–O stretches are at 1537 cm^{-1} and 1358 cm^{-1}.

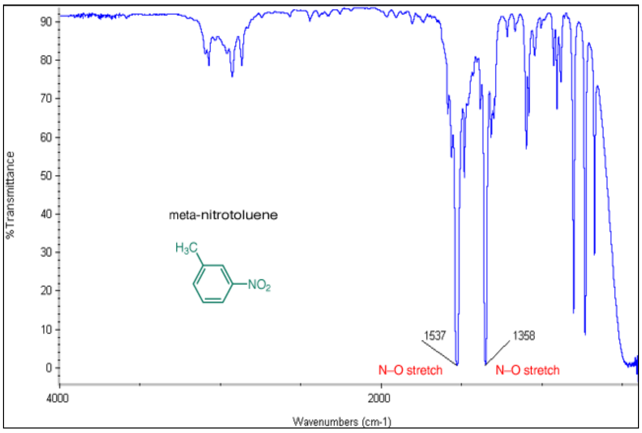

Fig 2: IR spectrum for meta-nitrotoluene

Table 1: Peak assignment in the FTIR spectrum of meta-nitrotoluene

Wave number, cm^{-1}	Functional grouping	Vibration mode
1537	N-O	Stretch
1358	N-O	Stretch

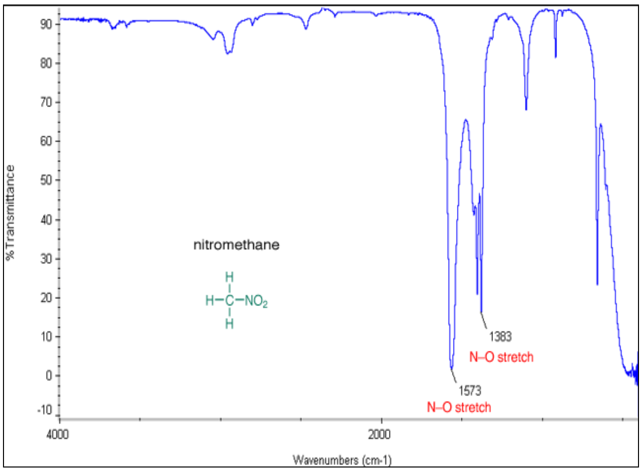

Fig 3: IR spectrum for meta nitromethane

Table 2: Peak assignment in the FTIR spectrum of meta nitromethane

Wave number, cm^{-1}	Functional grouping	Vibration mode
1573	N-O	Stretch
1383	N-O	Stretch

Conclusions

Nitrotoluene contains in IR only bands characteristic of functional groups: aromatics and nitro compounds. Nitromethane contains in IR only bands characteristic of functional groups: nitro compounds and alkanes.

Reference

1. Stanciu I. Journal of Science and Arts,2019:3(48):703–708.
2. Lluch C, Ronda JC, Galiá M, Lligadas G, Cádiz V. Biomacromolecules,2010:11:1646–1653.
3. Gaykar DV. Paint India,2001:7:55–60.
4. Clayton AM (Ed.). Epoxy Resin Chemistry and Technology. Marcel Dekker, 1988, 942.
5. Ahmed S, Ashraf SM, Naqvi F, Yadav S, Hasnat A. Journal of Polymer Materials,2001:18:53–60.
6. Bhunia HP, Nando GB, Chaki TK, Basak A, Lenka S, Nayak PL. European Polymer Journal,1999:38:1381–1391.
7. Shende PG, Dabhade SB. Polymer synthesis and applications. In: Vohra DK, Singh D, Singh P (Eds.). Proceedings of the National Seminar on Polymers, 1997, 104–110.
8. Aigbodion AI, Pillai CKS, Bakare IO, Yahaya LE. Indian Journal of Chemical Technology,2001:8:378–384.
9. Patel JV, Sony PK, Sinha VK. Journal of Polymer Materials,2001:18:103–110.
10. Pramanik S, Sagak K, Konwar BK, Karak N. Progress in Organic Coatings,2012:75:569–578.
11. Stanciu I. Rheological behaviour of biodegradable lubricant. Journal of Science and Arts,2019:3(48):703–708.
12. Stanciu I. Rheological investigation of soybean oil from soya beans. Journal of Science and Arts,2019:4(49):938–988.
13. Stanciu I. Modeling the temperature dependence of dynamic viscosity for rapeseed oil. Journal of Science and Arts,2011:1:55–58.
14. Stanciu I. Some methods for determining the viscosity index of hydraulic oil. Indian Journal of Science & Technology,2023:16(4):254–258.
15. Stanciu I. Rheological behavior of corn oil at different viscosity and shear rate. Oriental Journal of Chemistry,2023:39(2):335–339.
16. Stanciu I. Rheological characteristics of corn oil used in biodegradable lubricant. Oriental Journal of Chemistry,2023:39(3):592–595.
17. Stanciu I. Effect of temperature on rheology of corn (*Zea mays*) oil. Oriental Journal of Chemistry,2023:39(4):1068–1070.
18. Stanciu I. Study rheological behavior of rapeseed oils compared to mineral oil. Oriental Journal of Chemistry,2021:37(1):247–249.
19. Stanciu I. Influence of temperature on the rheological behavior of orange honey. Oriental Journal of Chemistry,2021:37(2):440–443.
20. Stanciu I. Rheological study of orange honey with influence on concentration. Oriental Journal of Chemistry,2021:37(4):864–867.