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Study of the composition of amines using IR spectroscopy

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Abstract
In this article we have determined by IR spectroscopy the chemical composition of the following amines: aniline, dimethylamine and trimethylamine. The absorption spectrum of aniline is comprised between the following wave numbers 3442cm^{-1} and 764cm^{-1}. The absorption spectrum of dimethylamine is comprised between the following wave numbers 3288cm^{-1} and 733cm^{-1}. The absorption spectrum of trimethylamine is comprised between the following wave numbers 3400cm^{-1} and 1214cm^{-1}.

Keywords: Anilina, dietilamina, trietilamina, compozitie

Introduction

Infrared spectrophotometry, IR deals with the study of vibrational and rotational (vibratory-rotational) spectra of molecules and the causes that cause molecular rotational and vibrational motion.

By coordinating ligands to the central atom, the formation of new metal-ligand bonds leads to a modification of the electronic structure, energy and symmetry of the compound. These changes affect the vibration of the ligand and consequently, in its spectrum, new vibrations characteristic of the newly formed compound appear.

The IR range is divided into three regions:

- far infrared (< 400 cm^{-1});
- mid-infrared (4000 – 400 cm^{-1});
- near-infrared (13,000 – 4000 cm^{-1}).

Most applications of IR spectroscopy include the mid-IR range;

- in the range 4000 - 1800 cm^{-1} generally a small number of bands appear,
- in the range 1800 - 600 cm^{-1} most bands appear and present the range of greatest interest.

This latter range is also called the "finger print" or "digital print" range
of the molecule. Certain groups in molecules produce bands called characteristic group frequencies, which greatly helps in the interpretation of IR spectra [1-5].

Normally each band in the IR spectrum can be attributed to vibrations of bonds between atoms, deformation of the molecule (in the plane and out of the plane), the movement of a group of atoms or some combined transitions.

An IR spectrum can contain hundreds of absorption bands, but not all of them should be interpreted.

Material and methods

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

Fig 1: Nicolet Avatar FTIR Spectrometer

Results and discussion

The N–H stretches of amines are in the region 3300-3000 cm^{-1}. These bands are weaker and sharper than those of the alcohol O–H stretches which appear in the same region. In primary amines (RNH_2), there are two bands in this region, the asymmetrical N–H stretch and the symmetrical N–H stretch.

Secondary amines (R_2NH) show only a single weak band in the 3300-3000 cm^{-1} region, since they have only one N–H bond. Tertiary amines (R_3N) do not show any band in this region since they do not have an N–H bond.

(A shoulder band usually appears on the lower wavenumber side in primary and secondary liquid amines arising from the overtone of the N–H bending band: this can confuse interpretation.)

The N–H bending vibration of primary amines is observed in the region 1650-1580 cm^{-1}. Usually, secondary amines do not show a band in this region and tertiary amines never show a Another band attributed to amines is observed in the region 910-665 cm^{-1}. This strong, broad band is due to N–H wag and observed only for primary and secondary amines.

The C–N stretching vibration of aliphatic amines is observed as medium or weak bands in the region 1250-1020 cm^{-1}. In aromatic amines, the band is usually strong and in the region 1335-1250 cm^{-1}.

Summary

- N–H stretch 3400-3250 cm^{-1}

o 1° amine: two bands from 3400-3300 and 3330-3250 cm^{-1}

o 2° amine: one band from 3350-3310 cm^{-1}

o 3° amine: no bands in this region

- N–H bend (primary amines only) from 1650-1580 cm^{-1}
- C–N stretch (aromatic amines) from 1335-1250 cm^{-1}
- C–N stretch (aliphatic amines) from 1250–1020 cm^{-1}
- N–H wag (primary and secondary amines only) from 910-665 cm_{-1}

The spectrum of aniline is shown below. This primary amine shows two N–H stretches (3442, 3360); note the shoulder band, which is an overtone of the N–H bending vibration. The C–N stretch appears at 1281 rather than at lower wavenumbers because aniline is an aromatic compound. Also note the N–H bend at 1619 [6-18].

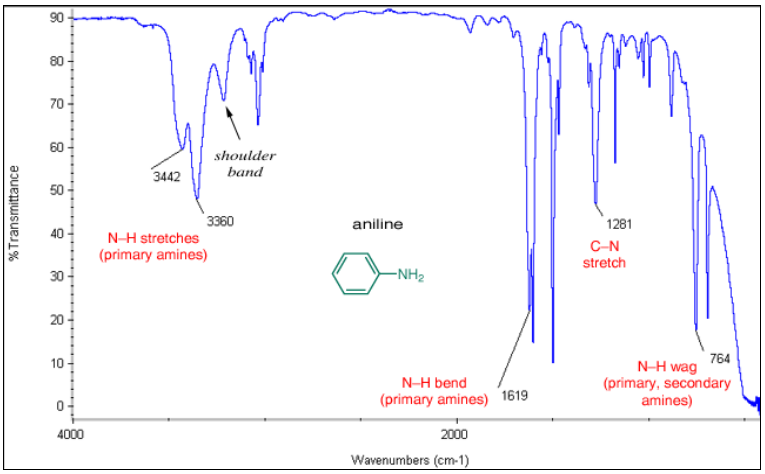

Fig 2: IR spectrum of aniline

Table 1: Peak assignment in the FTIR spectrum of aniline

Wave number, cm^{-1}	Functional grouping	Vibration mode
3442	N-H	stretches (primary amines)
3360	N-H	stretches (primary amines)
1619	N-H	bend (primary amines)
1281	C-N	stretch
764	N-H	wag(primary, secondary amines

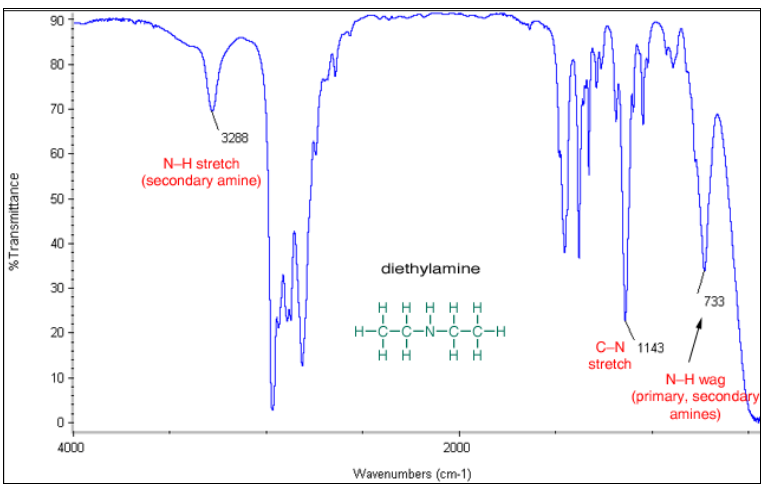

Fig 3: IR spectrum of diethylamine

Table 2: Peak assignment in the FTIR spectrum of diethylanine

Wave number, cm^{-1}	Functional grouping	Vibration mode
3288	N-H	stretch(secondary amines)
1143	C-N	stretch
733	N-H	wag(primary, secondary amines)

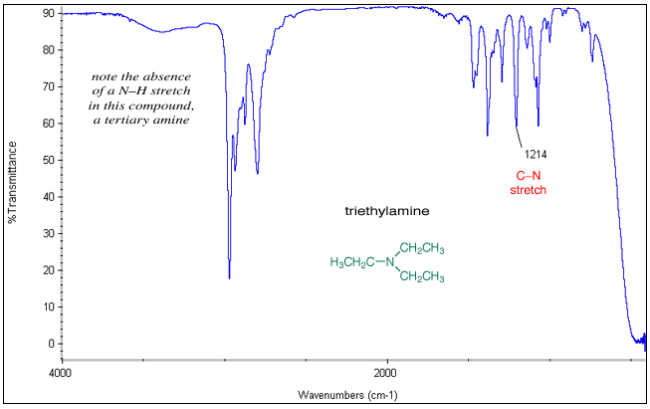

Fig 4: IR spectrum of triethylamine

Table 3: Peak assignment in the FTIR spectrum of triethylamine

Wave number, cm^{-1}	Functional grouping	Vibration mode
1214	C-N	stretch

Conclusions

Aniline contains in IR only bands characteristic of functional groups: primary, secondary amines, amides and aromatic amines. Dimethiamine contains in IR only bands characteristic of functional groups: primary, secondary amines, amides and alkanes. Trimethylamine contains in IR only bands characteristic of functional groups: aliphatic amines.

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