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Composition determined by IR spectroscopy of nicotine

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Abstract

The paper presents the study of the chemical composition of nicotine by Fourier transform infrared spectroscopy (FTIR). FTIR analysis allowed the identification of functional groups characteristic of the molecule, such as amine groups and C–H bonds of the pyridine and pyrrolidine rings. The results confirmed the molecular structure of nicotine and highlighted the potential of the FTIR method for the rapid identification and characterization of this compound. The study highlights the applicability of FTIR in organic chemistry and in the analysis of bioactive compounds, providing an efficient and non-invasive method for the detection of nicotine in various matrices.

Keywords: *spectra, composition, nicotine.*

Introduction

Nicotine (alpha 3 pyridyl-N-methylpyrrolidine) is a pyrrolidine alkaloid found in Nicotiana tabacum, family Solanaceae, and accounts for approximately 0.6–3.0% of the dry weight of tobacco. It can be used as an insecticide. At low concentrations (approximately 1 mg of nicotine absorbed), the substance acts as a stimulant in mammals and is the main factor responsible for addiction. According to the American Heart Association, nicotine addiction has historically been one of the most severe, while the pharmacological and behavioral characteristics that determine tobacco addiction are similar to those of heroin and cocaine addiction. The nicotine content of cigarettes has increased slowly over the years, and one study found that there was an average increase of 1.6% per year between 1998 and 2005. This was found for all major cigarette market categories [1-5].

Research from 2011 found that nicotine inhibits the enzyme-chromatin modification (class I and II histone deacetylases), which increases the ability of cocaine to cause addiction.

The oldest attestation of tobacco consumption is given by the identification of a 2.5 million year old tobacco block in Peru. The Mayans also used tobacco leaves for smoking. The Toltecs borrowed tobacco from their Mayan neighbors. Thus, two categories appear that use tobacco but for different purposes: those at the court of Montezuma who mixed tobacco with other resins and dried plants, the mixture being used in rituals. The second category is the Indians spread across the Mississippi River Valley, worshiping the Manitou who roll dried tobacco leaves in the form of a "crude cigar" cigarette

The colorless liquid is trainable with water vapor. Its isolation from the previously alkalized vegetable product is based on this property. Distillation takes place under vacuum to avoid decomposition. In contact with air it turns brown. It is miscible with water in any proportion at 60^0C and 120^0C. It is a levorotatory tertiary base, but its salts are dextrorotatory. At high temperatures on a platinum catalyst it can be reduced. The nitrogen atom in the pyrrolidine nucleus has a much more pronounced basic character than the nitrogen in the pyridine nucleus, a ring that is part of an aromatic structure. For this reason, the acidity constants have very different values:

-K_{a1} characteristic of N^+ pyridine has a value between 3.49-3.22

- K_{a2} characteristic of N^+ pyrrolidine has a value between 8.19-8.11

Each subunit is made up of 4 transmembrane segments numbered M1, M2, M3, M4, joined together by cellular

loops as follows: M1-M2, M2-M3 and M3-M4. In high doses, nicotine is a depolarizer of nicotinic receptors. In addition, it causes an increase in dopamine levels in the brain, due to the inhibition of MAO (monoamine oxidase) responsible for dopamine metabolism. However, it is not known for sure whether this action can be attributed to nicotine or other components of cigarette smoke (carcinogenic hydrocarbons). This action on dopamine is similar to that produced by cocaine and heroin, a reason why people smoke: maintaining a high level of dopamine, which determines the sensation of pleasure. Nicotine and its metabolites have been studied for the treatment of diseases such as: Parkinson's disease, Alzheimer's disease. Current research has shown that nicotine alone cannot develop cancer, it does not have mutagenic properties but by increasing the activity of acetylcholine, it leads to the prevention of apoptosis (programmed death) through which the body destroys certain types of cells, dead or mutated, thus developing into cancerous cells. Excitatory of the central and peripheral nervous system, in small doses inhibiting all sympathetic ganglia. Induces vomiting, decreases diuresis and increases intestinal motor activity. On the cardiac system it produces tachycardia, increases blood pressure and causes an increase in blood glucose [6-12].

Materials and methods

The primary material used in this analysis was a purified liquid sample of nicotine. The sample was stored in a sealed glass vial to prevent oxidation and contamination. Additional materials included potassium bromide (KBr) for pellet preparation (in the case of solid-state analysis), or alternatively, a liquid film cell with sodium chloride (NaCl) windows for liquid-phase measurements. Analytical-grade solvents such as ethanol were used if dilution was required. Laboratory equipment included an FTIR (Fourier Transform Infrared) spectrometer, micropipettes, a mortar and pestle (for KBr pellets), and clean glassware.

Prior to analysis, the IR spectrometer was calibrated according to the manufacturer's instructions to ensure accurate wavelength detection. A background spectrum was recorded to eliminate atmospheric interferences such as carbon dioxide and water vapor.

For liquid nicotine analysis, a small drop of the sample was placed between two NaCl plates to form a thin suitable for IR transmission. In the case of solid dispersion, a small amount of nicotine was mixed thoroughly with potassium bromide and pressed into a transparent pellet using a hydraulic press.

The sample was then placed in the IR spectrometer, and spectra were recorded over a range of 4000 to 400 cm^{-1}. This range covers the most relevant vibrational frequencies for organic functional groups. Multiple scans were performed to improve the signal-to-noise ratio, and the resulting spectra were averaged.

FT-IR spectrum were accomplished and recorded with Fourier-Transform infrared spectrophotometer (Bruker, Alpha ATR) between 4000 and 375 cm^{-1}, with resolution of 4 cm^{-1}.

Fig.1. *Infrared spectrophotometer Bruker*

Results and discussions

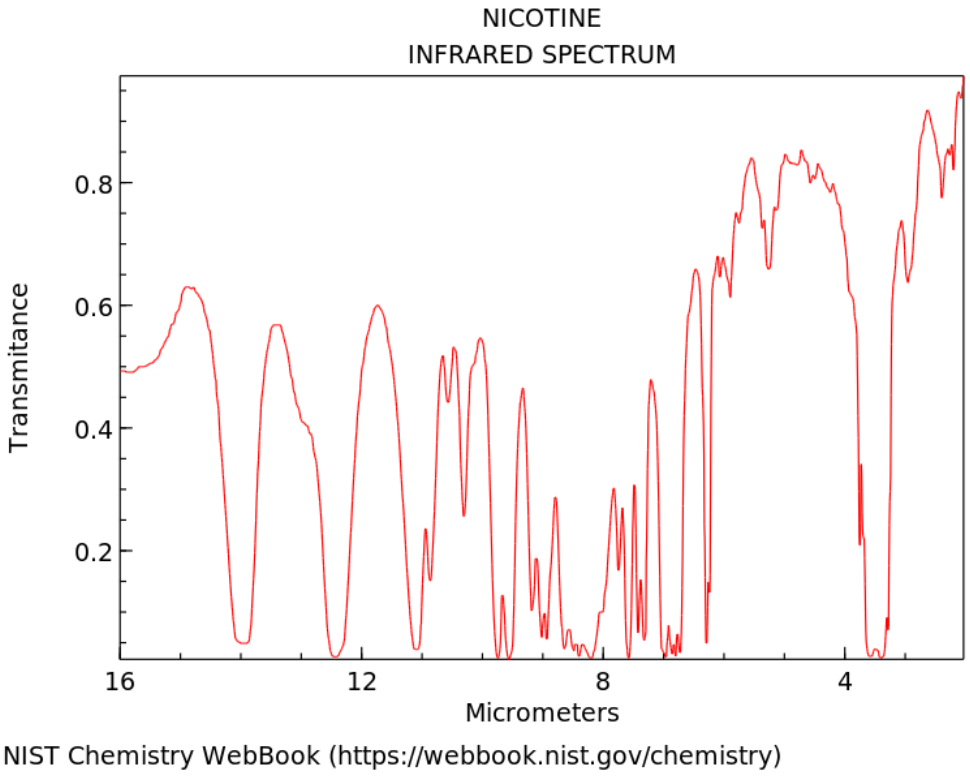

Fig.2. *IR spectrum of nicotine*

The infrared (IR) spectrum obtained for the nicotine sample provided detailed information regarding its molecular composition and functional groups. The analysis was carried out in the spectral range of 4000–400 cm^{-1}, which is characteristic for identifying organic compounds. The resulting spectrum exhibited several distinct absorption bands that are consistent with the known chemical structure of nicotine, confirming both its identity and relative purity.

Nicotine is a bicyclic compound composed of a pyridine ring and a pyrrolidine ring, containing multiple carbon–hydrogen (C–H), carbon–carbon (C=C), and carbon–nitrogen (C–N) bonds. The IR spectrum clearly reflected these structural features. One of the most prominent regions observed was between 3000 and 2850 cm^{-1}, where multiple absorption peaks were detected. These correspond to the stretching vibrations of aliphatic C–H bonds, primarily associated with the saturated pyrrolidine ring. Additionally, weak signals just above 3000 cm^{-1} indicated aromatic C–H stretching vibrations from the pyridine ring.

In the region between 1600 and 1450 cm^{-1}, several medium to strong absorption bands were present. These peaks are characteristic of C=C and C=N stretching vibrations within the aromatic pyridine ring. The presence of these peaks confirmed the aromatic nature of part of the nicotine molecule. The bands in this region were well-defined, suggesting a stable ring structure with no significant substitution or degradation.

Another important region in the spectrum was between 1200 and 1020 cm^{-1}, where strong absorption bands were observed. These are attributed to C–N stretching vibrations, which are indicative of amine groups. Nicotine contains two nitrogen atoms, both incorporated into ring systems, and these peaks supported their presence. The intensity and position of these bands were consistent with tertiary amines, particularly in the pyrrolidine ring.

Notably, there was an absence of a strong absorption band in the region around 3300–3500 cm^{-1}, where N–H stretching vibrations would typically appear. This observation is significant because it confirms that nicotine does not contain primary or secondary amine groups, but rather tertiary amines. This finding aligns with the known chemical structure of nicotine and further validates the accuracy of the spectral interpretation.

The fingerprint region (below 1500 cm^{-1}) also showed a complex pattern of peaks unique to nicotine. These peaks arise from various bending and stretching vibrations of the molecule's bonds and provide a distinctive spectral signature. Comparison of this region with reference spectra from spectral databases showed a high degree of similarity, confirming the identity of the analyzed compound.

In terms of purity, the spectrum did not reveal any unexpected peaks that could indicate the presence of contaminants such as water, alcohols, or other organic impurities. For example, there were no broad O–H

stretching bands around 3400 cm^{-1}, which would suggest moisture contamination, nor were there carbonyl (C=O) peaks near 1700 cm^{-1}, which could indicate oxidation products. This suggests that the nicotine sample analyzed was of high purity and had not undergone significant degradation.

Minor baseline fluctuations and very weak peaks were observed in some regions of the spectrum. These could be attributed to instrumental noise, atmospheric interference (e.g., residual carbon dioxide or water vapor), or trace impurities at levels below significant concern. However, these did not interfere with the main spectral features or the overall interpretation.

The results demonstrate that IR spectroscopy is a reliable and effective method for confirming the composition of nicotine. By analyzing the presence and absence of specific functional group vibrations, it is possible to verify both the structure and purity of the compound. The technique's non-destructive nature and relatively simple sample preparation make it particularly useful for routine laboratory analysis. [13-19].

Conclusions

The FTIR spectrum allowed the identification of the main functional groups in the nicotine molecule, including primary and secondary amines and C–H bonds of the pyridine and pyrrolidine rings. Analysis of the characteristic bands confirms the known chemical structure of nicotine ($C_{10}H_{14}N_2$) and the presence of reactive groups. FTIR has proven to be a rapid, non-invasive and reproducible method for the identification and characterization of nicotine in various samples. The study demonstrates the potential of FTIR in the research of bioactive compounds, the analysis of tobacco substances and the monitoring of the presence of nicotine in biological or industrial matrices.

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