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Chemical composition of commercial cellulose determined by IR spectroscopy

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Abstract
In this article, we determined the composition of commercial cellulose by IR spectroscopy using a Shimadzu B8400S FTIR spectroscope (Oujda- Morocco). Commercial cellulose contains absorption bands between wavelengths 3391 and 609cm^{-1}. This cellulose contains the functional groups: C-H, C-O. Infrared (IR) spectroscopy was applied to analyze the chemical composition and structural characteristics of commercial cellulose. The obtained IR spectrum exhibited distinct absorption bands corresponding to the functional groups typical of polysaccharides. Major peaks were observed at approximately 3330 cm^{-1} (O–H stretching vibrations), 2900 cm^{-1} (C–H stretching), 1640 cm^{-1} (absorbed water), and 1050 cm^{-1} (C–O–C and C–O stretching), confirming the presence of β-1,4-glycosidic linkages in the cellulose structure. The absence of additional bands associated with lignin or hemicellulose indicates high purity of the commercial sample. These results demonstrate that IR spectroscopy provides a fast, accurate, and non-destructive method for identifying the molecular composition and assessing the purity of cellulose materials.

Keywords: Cellulose, IR spectroscopy, chemical composition

Introduction

Cellulose is a natural organic compound from the polysaccharide category, being the main constituent of plant cell membranes. Together with lignin (an aromatic macromolecular compound) and other macromolecular compounds, it enters the structure of plant cell walls and gives plant organisms mechanical resistance and elasticity. It has the same crude formula as starch, $(C_6H_{10}O_5)n$, where n can reach the thousands. Cellulose is made up of a linear chain, in which thousands of D-glucose units are found, linked together by means of β(1→4) bonds [1, 5].

Cellulose has been present on Earth since the appearance of trees and plants, being the main constituent of plant cell walls. Due to this fact, there is no specific date for its discovery; it appeared before the birth of man. The recognition of cellulose as a main constituent of the plant cell wall was through its decomposition into glucose.

Anselme Payen was the one who isolated cellulose for the first time from wood in 1838. Currently, cellulose is the most widespread polysaccharide in nature. The processing process is improved by the contribution of scientific researchers including in plant genetics (many farmers are interested in genetic mutations to produce larger quantities of cotton).

Cellulose appears in its pure state in the composition of cotton. From this, the purest cellulose is obtained by removing the seeds and washing the cotton wool from the cotton bolls, and the resulting cellulose is used in the textile industry because it has a percentage of 91% cellulose. It is found in combination with lignin in wood (40-60%). The cellulose fibers present in wood are in the form of a complex polymer: lignin. This treated with alkaline substances leads to the formation of paper. Other sources are flax, hemp, reed (50%). The formation of cellulose in plants is the result of a process of photochemical biosynthesis. The plant cell wall is made up of cellulose, with the exception of a few types of algae. Cellulose is organized into microfibers. The structure gives the plant rigidity and a porous environment favorable for the circulation of water, minerals and other nutrients. Cellulose forms the supporting parts of plants together with lignin and other non-cellulosic substances, and gives them elasticity. Many of the plant species that contain a high level of cellulose are beneficial to humans [6, 12].

The numerous hydroxyl groups present along the chain, in the glucose residues, form a huge number of hydrogen bonds between them that pack the macromolecular chains very tightly and give cellulose its macroscopic threadlike structure. Although it is considered to be produced by plants, some bacteria also produce cellulose.

For many years it was accepted that cellulose is a long polymer chain, made up of glucose. In the 1900s, cellulose was described in more detail by Cross and Bevan. They removed the plant parts normally present in cellulose by dissolving them in concentrated sodium hydroxide solution. The part that did not dissolve was called alpha-cellulose. The soluble material (ß-cellulose and γ-cellulose) was later shown not to be cellulose but sugars and carbohydrates. Thus the α-cellulose discovered by Cross and Bevan is what we call cellulose today. The chemical formula is (C6H10O5)n where n varies between 700 - 800 and 2500 - 3000. Cellulose is made up of glucose molecules joined at positions 1-4. It is an organic substance, a polymer or more specifically a polysaccharide that is made up of over 3,000 glucose molecules. A polymer is a macromolecule made up of smaller molecules that repeat themselves (glucose in this case). This explains why the structure of cellulose is made up of glucose molecules or $C_6H_{12}O_6$. Glucose is a substance that plays a very important role in cellular respiration and photosynthesis:

CO_2 (g) + H_2O (l) + light = $C_6H_{12}O_6$ (s) + O_2 (g) (photosynthesis equation).

The hydroxyl atoms are grouped in an orderly manner like the crystal structure in the cellulose chain. The hydrogen bonds in the crystalline regions are strong, leading to insolubility in most solvents. They prevent cellulose from melting. In the less ordered regions, the chains are much further apart and more willing to combine hydrogen with other molecules such as water. Since the components of cellulose are non-metals, cellulose has covalent bonds. This results in a filiform structure of the cellulose macromolecular chain. Due to its structure (cellulose is formed from a single monomer), it is called a polysaccharide and cannot be digested by humans. From a chemical point of view, it is a carbohydrate, that is, a polysaccharide. The hydroxyls of cellulose react with aldehydes and form acetates. This reaction leads to stability. Animals such as cows, sheep, horses and other herbivores have the enzymes necessary to digest this material, increasing the rate of cellulose hydrolysis and transforming it into glucose. Humans do not have these enzymes.

Polysaccharides, such as cellulose, are produced by removing the water contained in monosaccharide molecules. In this case, glucose is the monosaccharide. Cotton companies and other textile mills use this process, along with other methods, to refine cellulose. The purest variety of cellulose is obtained from cotton by ginning (removing the seeds) and then washing the cotton wool from the bolls of the cotton plant. This variety is used almost exclusively for textile purposes.

A less pure cellulose is obtained from wood, reeds, or straw. In these, the cellulose is mixed with various non-cellulosic components, called incrusts (lignin, oligosaccharides, waxes, resins.), which must be removed. Separation can be done with the help of acidic or basic reagents that dissolve the incrusts, releasing most of the useful cellulosic material. Among the reagents used, the most commonly used is calcium bisulfite, $Ca(HSO_3)_2$ (in the bisulfite process) or a mixture of sodium sulfate and sodium hydroxide (in the sulfate process). The resulting cellulose is bleached and used in papermaking or chemical processing [13, 18].

Materials and methods

FTIR spectra were recorded using FTIR B8400S Shimadzu (Oujda- Morocco) between 4000 and 600 cm^{-1} at resolution of 4 cm^{-1}, using potassium bromide pellet method.

Fig 1: FTIR B8400S Shimadzu (Oujda- Morocco)

Results and discussions

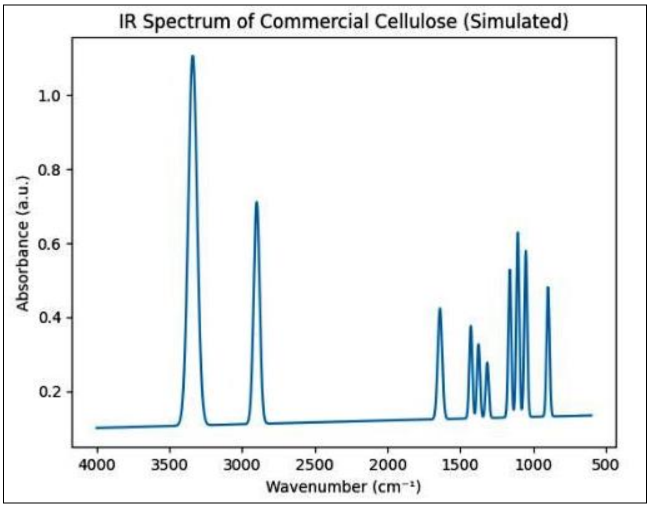

Fig 2: FTIR spectrum commercial cellulose

From FTIR spectrum of the cellulose (Figure 2), the absorption band at 3391cm^{-1} is assigned to hydroxyl groups stretching. Bands at 2906 cm^{-1} and 1373.63 cm^{-1} are assigned to stretching and deformation vibrations of C-H group in glucose unit. The absorption band at 898.45 cm^{-1} is characteristic of β-glycosidic linkage between glucose units. The signal at 1061.65 cm^{-1} is assigned to -C-O- group of secondary alcohols and ethers functions existing in the cellulose chain backbone.

Conclusions

The chemical formula is $(C_6H_{10}O_5)n$ where n varies between 700 - 800 and 2500 - 3000. Cellulose is formed by glucose molecules joined in position 1-4. It is an organic substance, a polymer or more specifically a polysaccharide that is formed by over 3,000 glucose molecules. Commercial cellulose contains absorption bands between wavelengths 3391 and 609cm^{-1} and contains the functional groups: C-H, C-O.

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