International Journal of Advanced Research and Development
www.multireviewjournal.com
ISSN: 2455-4030
Received: 25-11-2025, Accepted: 24-12-2025, Published: 08-01-2026
Volume 11, Issue 1, 2026, Page No. 1-2

Composition of acetic acid determined by IR spectroscopy

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Abstract
In this article, we determined the composition of acetic acid by IR spectroscopy using a Bruker spectroscope. The wavelength range in which absorption bands appear is between 3400 cm^{-1} and 450 cm^{-1}. The bands observed in the spectrum, especially in the regions 1700–1750 cm^{-1} (C=O) and 2500–3300 cm^{-1} (O–H), confirm the chemical structure of acetic acid and the integrity of the sample.

Keywords: Spectroscopy, IR spectrum, acetic acid

Introduction

Better known as vinegar, acetic acid is an organic chemical compound with the chemical formula CH_3COOH. It is one of the simplest carboxylic acids. Acetic acid is a colorless liquid with a characteristic pungent odor and sour taste. It is soluble in water, alcohol, and ether, and is found naturally in some fermented products.

Acetic acid can be produced by several methods, including the fermentation of ethyl alcohol. The chemical industry produces mostly synthetic acetic acid, which is used in various applications such as the production of plastics, textiles, and solvents. Due to its chemical and physical properties, acetic acid is used in many fields, such as the food industry, pharmaceuticals, cosmetics, cleaning, and agriculture. Acetic acid is mainly used in the food industry for the production of pickles, condiments, sauces, and dressings. In addition, acetic acid is used in the household as a cleaning and disinfecting agent, being effective against bacteria and fungi. It is also used in agriculture in pesticides and herbicides.

Acetic acid has the chemical formula CH_3COOH. The acetic acid molecule consists of a methyl group (CH_3) bonded to a carboxyl group (COOH), which gives the compound its acidic properties [1, 5].

Acetic acid is a colorless liquid with a pungent and characteristic odor. It has a melting point of 16.6 degrees Celsius and a boiling point of 118.1 degrees Celsius. Acetic acid is soluble in water, alcohol, and ether, due to the presence of the carboxyl group, which forms hydrogen bonds with other molecules.

Acetic acid is a weak acid, having a pKa of 4.76, which means that it partially dissociates in aqueous solution, forming acetate ions (CH_3COO^-) and protons (H^+). Acetic acid is a polar molecule, due to the difference in electronegativity between the carbon, oxygen, and hydrogen atoms. The presence of hydrogen bonds between acetic acid molecules results in relatively high surface tension and viscosity, as well as high melting and boiling points compared to other compounds of similar size [6, 11].

Acetic acid has multiple health benefits. One of the most important is related to blood sugar control. Studies show that consuming acetic acid can help delay the release of glucose into the blood and increase insulin sensitivity, especially in people diagnosed with type 2 diabetes or prediabetes. Apple cider vinegar is a popular source of acetic acid, which can be added to salads or drunk, diluted in water.

In addition to its benefits for blood sugar control, acetic acid also has antimicrobial and antibacterial properties. It can destroy certain bacteria and fungi that are potentially harmful to the body. Therefore, it can be used in the treatment of skin infections and in the prevention and treatment of colds or flu. Acetic acid can also improve gut health by killing harmful bacteria and fungi and promoting the growth of beneficial bacteria.

Consuming acetic acid can also aid in weight loss. It can suppress appetite, reduce fat storage, and improve metabolism.

In addition to the benefits mentioned above, acetic acid may also have beneficial effects on heart health. It can reduce bad cholesterol (LDL) and triglycerides, and improve endothelial function. These effects may help prevent cardiovascular disease [2].

In conclusion, consuming acetic acid can provide multiple health benefits, but it should be consumed in moderation. As a precaution, it is important not to consume too much vinegar, as it can cause irritation to the digestive tract [12, 17].

Materials and methods

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}.

The FT-IR bands of CH_3COOH (Fig. 2) [18]. The spectrum can be divided into three distinctive regions. High energy bands, around 3,400 and 2,935 cm^{-1} correspond to ν(O–H) and ν(C–H) stretching vibrations, respectively. On the low energy side of the spectrum, three sets of bands appear, corresponding to rocking $\rho(CH_3)$ (around 1,000 cm^{-1}), stretching ν(C–C) (around 950 cm^{-1}), and deformation δ(COO) (between 450 and 700 cm^{-1}) vibrations, respectively. On the middle energy range, three sets of bands (δ(OH), ν(COO), and $\delta(CH_3)$) contribute to the FT-IR spectrum: one set, located at 1,700 and 1,600 cm^{-1}, corresponds to deformation mode δ(OH) of the water molecule. Another set is the set characteristic for the strong bands of acetate ligands appearing around 1,500 cm^{-1}. Four kinds of coordination of acetate groups are generally considered, according to the literature [19]: monodentate (I), chelating (II), bridging (III), and polymeric (IV).

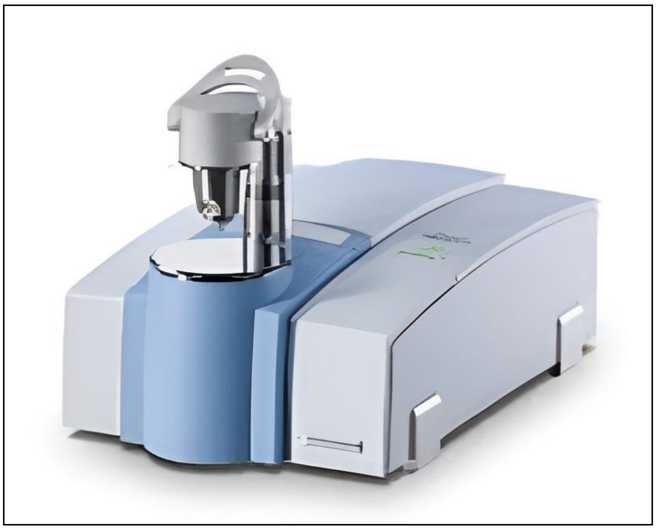

Fig 1: Infrared spectrophotometer Bruker

Result and discussion

Figure 2 shows the FTIR spectrum of acetic acid.

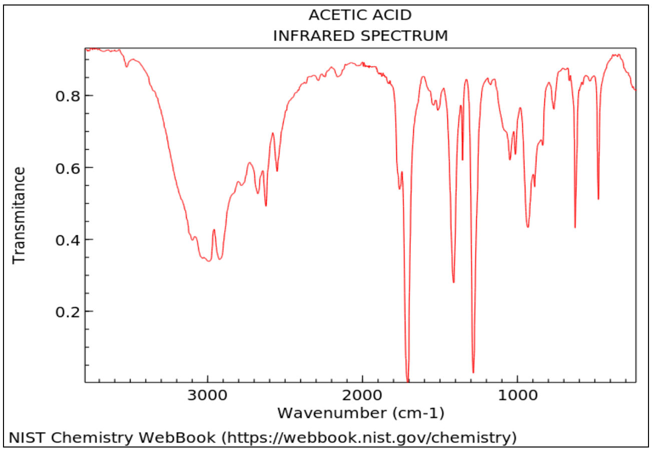

Fig 2: IR spectrum of acetic acid

Conclusion

FTIR spectroscopy allowed the identification of functional groups characteristic of acetic acid, especially the carboxyl group (-COOH). The bands observed in the spectrum, especially in the regions 1700–1750 cm^{-1} (C=O) and 2500–3300 cm^{-1} (O–H), confirm the chemical structure of acetic acid and the integrity of the sample. FTIR analysis has proven to be rapid, non-destructive and efficient for the qualitative characterization of acetic acid. The method can be used for quality control and verification of the purity of acetic acid in chemical laboratories and industrial applications. The obtained results provide a reference basis for further studies on the interactions and stability of acetic acid in different environments.

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