

## Composition determined by IR spectroscopy of chloroform

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### Abstract

In this article, we determined the composition of chloroform by FTIR spectroscopy using a Perkin Elmer Spectrum GX spectrometer. Chloroform contains absorption bands between 1312 and 757 $\text{cm}^{-1}$  and contains the following functional groups: —COO, —CONH, C-H and  $\text{CHCl}_3$ . Chloroform (trichloromethane,  $\text{CHCl}_3$ ) is a halogenated organic compound, belonging to the class of chloromethanes, characterized by a molecular structure formed by a carbon atom bonded to a hydrogen atom and three chlorine atoms. This electronic distribution gives the molecule relative stability, low polarity and high volatility, properties that have determined its historical uses in extraction, laboratory and medicine. Currently, its role is being reevaluated due to toxicological risks, potential carcinogenicity and bacterial formation of phosgene under certain conditions. Contemporary studies focus on its behavior in the environment, atmospheric degradation mechanisms, as well as the impact on industrial health and safety. Understanding the chemical composition and physical properties of chloroform remains essential for risk assessment and its responsible management in modern applications, in the context of the transition to safer solvents and sustainable practices.

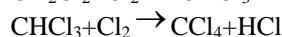
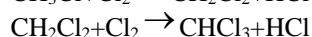
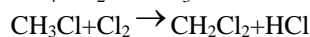
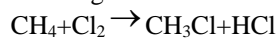
**Keywords:** chemical composition, chloroform, IR spectroscopy

### Introduction

Chloroform or trichloromethane is a chlorinated hydrocarbon with the chemical formula  $\text{CHCl}_3$ . It was discovered in 1831 by Justus von Liebig, Samuel Guthrie and Eugène Soubeiran.

Trichloromethane is a colorless, nonflammable liquid with a sweet odor. It has a higher density than water, being soluble only in organic solvents. Chloroform vapors cause loss of consciousness and reduced sensitivity to pain when inhaled. Due to its toxic effect on the heart, liver and other internal organs, it is no longer used as a narcotic. It is also assumed to have a carcinogenic effect. Chloroform decomposes in the presence of oxygen in the presence of light, forming phosgene, chlorine and hypochlorous acid ( $\text{HClO}$ ). Commercially available chloroform is a mixture with 0.5–1.0% ethanol as a stabilizer<sup>[1, 5]</sup>.

On an industrial scale, chloroform is obtained by heating chlorine with methane or methane chloride at 400–500 °C, resulting in a substitution reaction:



The end result is a mixture of methane chlorides that are separated by fractional distillation.

Chloroform is mainly used as a diluent and in the production of chlorofluorocarbons which are responsible for the formation of ozone holes in the upper atmosphere. Deuterated chloroform, ( $\text{CDCl}_3$ ), being called chloroform-deuterium is used in nuclear magnetic resonance (NMR) spectroscopy.

Some anaerobic bacteria use chloroform for respiration, in a process called respiration converting it to dichloromethane [6, 12].

### Materials and methods

Fourier transform infrared (FTIR) spectra were recorded on a Perkin Elmer Spectrum GX spectrophotometer using chloroform as solvent.



Fig 1: Perkin Elmer Spectrum GX spectrophotometer

### Results and discussions

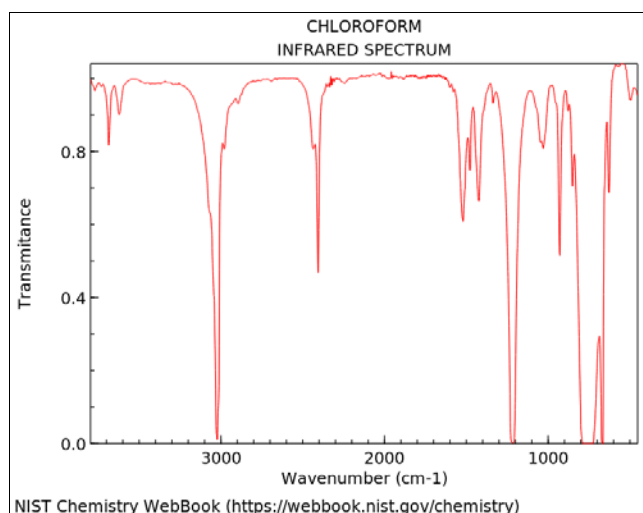


Fig 2: Spectral IR al cloroformului

The FTIR spectrum of 5 showed a peak at  $1735\text{ cm}^{-1}$  due to the carbonyl stretching frequency of ester ( $-\text{COO}$ ) and at  $1694\text{ cm}^{-1}$  due to the carbonyl stretching of amide ( $-\text{CONH}$ ) (Fig. 2). The IR spectrum of chloroform is shown as below: the signal at  $3012\text{ cm}^{-1}$  is for C-H stretching of the chloroform. The signal at  $1200\text{ cm}^{-1}$  are for C-H bending of the chloroform. The signal at  $757\text{ cm}^{-1}$  is for  $\text{CHCl}_3$  stretching of the chloroform<sup>[13, 19]</sup>.

### Conclusions

Chloroform contains absorption bands between  $1312$  and  $757\text{ cm}^{-1}$  and contains the following functional groups:  $-\text{COO}$ ,  $-\text{CONH}$ , C-H and  $\text{CHCl}_3$  and were determined with the Perkin Elmer Spectrum GX spectrometer. Chloroform, chemically defined as trichloromethane ( $\text{CHCl}_3$ ), is a simple but significant molecule in the chemistry of halogenated compounds. Its structure, consisting of a carbon atom bonded to three chlorine atoms and one hydrogen atom, determines distinct physical properties such as high volatility, relative stability, and low polarity. This composition has been the basis of its historical uses as a solvent and anesthetic agent, although toxicological risks and health impacts have led to strict regulation of its modern application. Overall, understanding the composition of chloroform highlights the relationship between molecular structure and its behavior in chemical, industrial, and environmental applications, emphasizing the need for responsible management of this compound.

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