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Chemical composition of glycerol determined by IR spectroscopy

Ioana Stanciu*
Faculty of Chemistry, Department of Physical Chemistry, University of Bucharest, Elisabeta Blvd, Bucharest, Romania

Abstract
Glycerin, also known as glycerol, is an organic compound of the trihydric alcohol type with the chemical formula $C_3H_8O_3$, characterized by the presence of three hydroxyl groups (-OH) attached to a chain of three carbon atoms. This work aims to analyze the chemical structure, physicochemical properties and reactivity of glycerin, highlighting its role in the synthesis of esters and in the formation of triglycerides. The study highlights its high solubility in water, hygroscopic nature and applicability in various industrial and pharmaceutical fields. The results obtained provide a detailed understanding of the molecular characteristics of glycerin and contribute to its better utilization in practical chemistry.

Keywords: Glycerol, spectroscopy, chemical composition, FTIR

Introduction

Glycerol (chemical formula $CH_2OHCHOHCH_2OH$) also called glycerin is the simplest trihydric alcohol with a molar mass of 92.09. It is a syrupy, colorless, sweet liquid, soluble in water and alcohol with a boiling point of 290 °C. Glycerol evaporates and freezes slowly, for example, an 80% solution freezes at -20.3 °C. In the form of fatty acid esters (glycerides), it is the basic component of animal and vegetable fats, including phospholipids and plasmalogens.

Glycerol is obtained by saponification of fats, and in industry from the waters remaining from soap manufacturing, by glycolic fermentation of sugars. Synthetically it is obtained from propylene from petroleum cracking. It is used to obtain nitroglycerin, synthetic resins, in tanning, paper manufacturing, in the food industry, in cosmetics and pharmaceuticals [1-5].

Glycerin was discovered by Scheele in 1780 in the waste water from the saponification of fats. It is still produced on a large scale by this method today. Another manufacturing method is based on the fermentation of glucose with brewer's yeast in the presence of sodium sulfite. About modern synthesis processes, starting from propene in petroleum gases. Glycerin crystallizes slowly. When kept for a longer period of time at a temperature below 0 °C, it forms crystals with a m.p. of 20 degrees. Glycerin is used in the explosives industry, in pharmacy and cosmetics, in the leather industry and for the manufacture of plastics. Glycerin is hygroscopic, it absorbs water vapor from the atmosphere until an equilibrium is established.

Glycerin (glycerol) has a boiling point of 290 °C, being completely stable up to this threshold, only in the absence of molecular oxygen in the environment (anaerobic conditions). Between the flash point (180 °C) and the boiling point, glycerin, in the presence of oxygen (aerobic conditions), releases variable amounts of acrolein, a toxic and polluting substance. Acrolein is no longer formed from glycerol at temperatures above 290 °C, regardless of whether atmospheric oxygen is present or absent. Glycerin evaporates and freezes slowly, for example, the 8.0% solution freezes at -20.3 °C. In the form of fatty acid esters (glycerides), it is the basic component of animal and vegetable fats from which it is obtained by saponification and in industry from the waters remaining from soap manufacturing, by glycolic fermentation of sugars [6-12].

Glycerin is a liquid substance, relatively viscous, with a density higher than that of water, colorless, with a sweet taste and odorless. It is easily soluble in water and in ethyl alcohol. In turn, glycerol is a good solvent for various substances, being used, especially in gemotherapy, phytotherapy and homeopathy for the extraction of active principles of plant origin.

Glycerol in the human body derives from the enzymatic hydrolysis of glycerides in food (see digestion and absorption of lipids). Under the influence of specific enzymes (lipases), the hydrolysis reaction takes place, which, being reversible, leads to both the synthesis of glycerides and their degradation.

Glycerin is also used in the production of alcoholic beverages because of its sweet taste. Archived April 12, 2019, at the Wayback Machine. It is a moisturizing agent found in countless cosmetic products for skin and hair care and hygiene. It facilitates water retention in the skin tissue, is emollient and softening, and protects hair from dehydration [7-17].

Materials and methods

The Carry 660 FTIR spectrophotometer was used for the analysis of the refined glycerol. The FTIR analysis of the crude and refined glycerol was performed by using Diamond Crystal over a scanning range of 4000-650 cm^{-1}.

Fig 1: Carry 660 FTIR spectrophotometer

Results and discussions

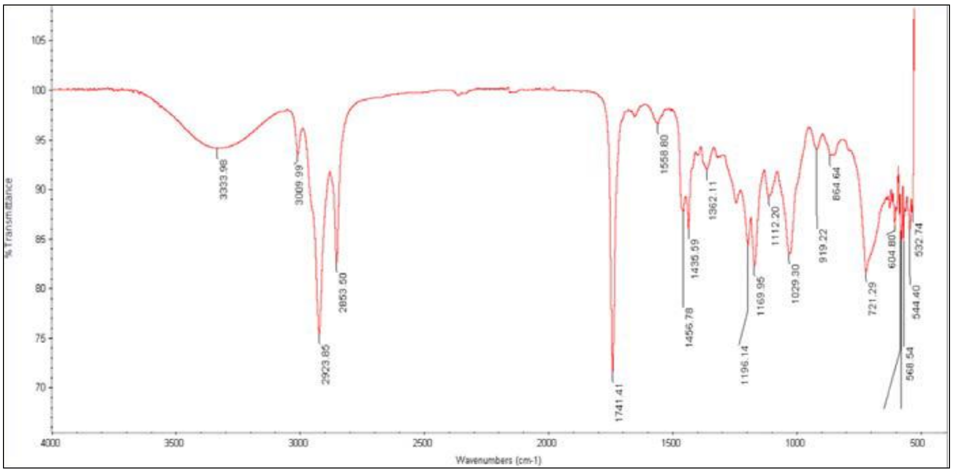

Fig 2: IR Spectrum of crude glycerol

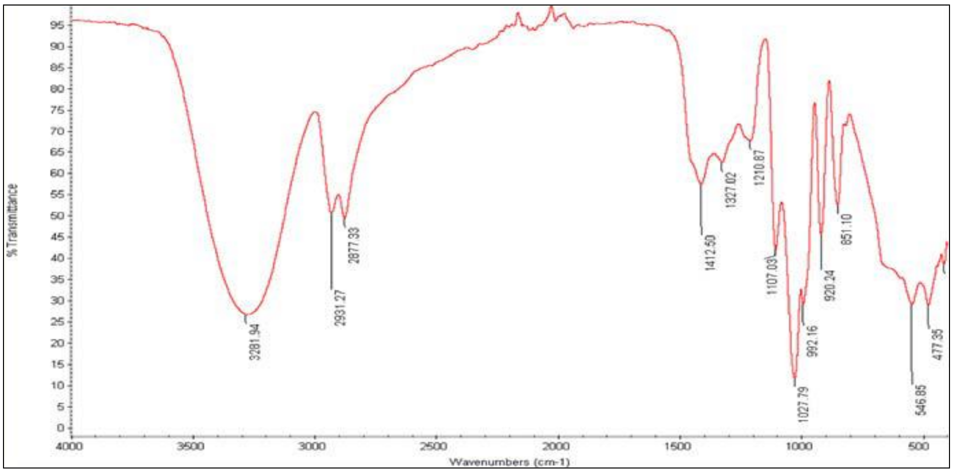

Fig 3: IR Spectrum of refined glycerol

The FTIR spectrum of the crude glycerol was complex (Figure 2) showing peaks of several functional groups. O-H stretching frequency was observed at 3321.78 cm-1 while a strong peak at 1739.61 cm-1 was due to the C=O stretching of esters present in the crude glycerol. O-H bending was observed at 910.22 cm-1, while the COO group related to soap impurities showed a peak at 1548.80 cm-1, representing dissolved salts in the crude glycerol. A peak at 3009.99 cm^{-1} could be attributed to C=C present in the alkyl part of the fatty acid chain [18]. FTIR spectrum of the refined glycerol is shown in Figure 3. From the spectrum, it was depicted that the functional groups present in this spectrum were alike to those described in literature. The FTIR spectrum of the refined glycerol showed O-H stretching at 3265 cm^{-1} while C-H stretching was revealed by the peaks in the region of 2810-2950 cm^{-1}. The C=O stretching band present in the crude glycerol at 1655 cm-1 was absent in the refined glycerol spectra.

The peak at 1560 cm^{-1} was also absent in the refined glycerol indicating the removal of the salts. Bending of the C-O-H group was also observed in the region of 1400 to 1420 cm^{-1} of the C-O stretching of the primary alcohol, which is shown at 1112 cm^{-1} [19].

Conclusions

Intense and broad bands in the 3200–3600 cm^{-1} region confirm the presence of multiple hydroxyl groups, characteristic of a trihydric alcohol. Bands in 2850–2950 cm^{-1} corresponding to the stretching vibrations of the C-H bonds in the methyl and methylene groups, specific to the carbon chain. C-O stretching vibrations in 1050–1150 cm^{-1} confirm the presence of primary and secondary alcohols. The IR spectrum confirms the chemical formula $C_3H_8O_3$ and the nature of a trihydric alcohol, highlighting that glycerin can form hydrogen bonds and has a hygroscopic character. The IR spectrum can be used for the identification and purity of glycerin in chemical and industrial laboratories.

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