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QUANTITATIVE ANALYSIS OF PHARMACEUTICAL POLYMORPH POLYSTYRENE, POLYCARBON, POLYMETHYLMETHACRYLATE, POLYETHYLENE WITH RAMAN SPECTROSCOPY

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Abstract

It involves the partitioning of light or microwaves according to their wavelength, which constitutes a spectrum. Proposed research analyses interpret the observed data set in accordance with the experimental procedure. The numerical quantitative analysis employs least squares methods to assess the composition and error. Based on the preceding analysis, we performed an estimation and standard deviation analysis on the quantified data to ascertain the findings of the research. This research paper examined various varieties of Raman spectroscopies utilized in the pharmaceutical industry and other sectors. This article discussed the benefits and drawbacks of various polymers and crystal structures, including polystyrene (PS), polycarbonate (PC), polymethylmethacrylate (PMMA), polyethylene (PE), polyethylene terephthalate (PET), and polypropylene (PP).

Key words: polymorph, raman spectroscopy, drug.

1. Introduction

Pharmaceutical (medicinal) chemistry is concerned with the design (drug design) and synthesis of biologically active molecules [1]. The aim is to gain new chemical molecules that could enable the discovery of new pharmaceuticals or optimize already known drug structures, thereby to expand the portfolio of chemical drugs [2]. Although organic chemistry plays a crucial role, only knowledgeable pharmaceutical chemists are able to work effectively in a highly interdisciplinary environment and interact with scientists in other disciplines, such as molecular biology, structural biology, pharmacology, physical chemistry, biochemistry, pharmacokinetics, pharmaceutical technology, toxicology or with experts from the field of translational medicine, etc [3,4].

When the same molecule may exist in a number of crystallographic forms, this phenomenon is referred to as diversity [5]. Various problems arise in terms of physical properties such as volume, sublimation temperatures and melting, density, properties like rate of dissolution, etc [6]. As a result, the compound's bioavailability is variable and dependable on the form of the crystal. When the molecule can be used as a solvate, then the term pseudo polymorphism is used with the most common being hydrates [7]. An example of pseudo polymorphism is; that in the theophylline tables, the hydration state changed. The theophylline is present in monohydrate or, the crystalline hydrate because in terms of changes in humidity and temperature, the water is adsorbed and desorbed. In the pharmaceutical manufacturing area, the use of polymorph is very vital [8]. Therefore, the rates of determined physiological dissolution and the control of them are very critical. The forms of polymorph are used in vibration spectroscopy by low-wavenumber vibrational (phonon) modes. These are basically accessible by terahertz or Raman spectroscopy.

In this work qualitative analysis of various polymorph compounds has been done using raman spectroscopy.

2. Material and method

Every component and pharmaceutical product was obtained either from retail pharmacies in the immediate area or directly from pharmaceutical manufacturers. The analytical grade of solvents was employed in this experiment. DSC and X-ray diffraction were used to characterize the starting material as well as the crystal forms that were created. This was done in order to confirm the identity of the crystal phases by comparing them to the previous research. The pure polymorphs will be geometrically mixed together to produce different binary mixtures. Although it covers a reasonable amount of ground over the whole concentration range, the mixing technique places more of an emphasis on lower concentrations of various forms. In the end, count not more than 20 samples, including the initial ingredients, was utilized.

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2.1. DATA COLLECTION TECHNIQUES

Every computation was worked out on a personal computer outfitted with Microsoft "Windows XP, an Intel Pentium 3 GHz CPU", and 768 megabytes of random-access memory (RAM). "For the OSC, SNV, and MSC transformations", as well as the fitting of the PLS models, the "Simca-P v.9 (Umetrics AB)" was utilized. On the other hand, the Kennard-Stone routine of the "ChemoAC toolbox for Matlab (Matlab 6.5, Mathworks Inc.)" was utilized for the separation of the data into uniform training and test subsets. The predictive performance was evaluated based on the *root mean squared error* of cross-validation, calibration, and prediction. This error was computed by using the following formula:

$$\text{RMSE} = \sqrt{\frac{\sum_{i-1}^{\pi} (y_i - \bar{y}_i)^2}{n}}$$

3.0 Result and discussion

3.1. Polystyrene (PS):

The below image shows the structural formula of polymer of **styrene**, which is called as Polystyrene (PS). A type of thermoplastic reactive polymeric with a helical core is paraffin. It becomes a glossy solid at ambient temperature, but as it reaches the glass transition point of roughly 100 °C, it gains flexibility and may flow. Chemically resistant to many hostile substances, it is solubility in certain aromatic compounds like the chemicals benzene as well as inorganic chlorinated ones such as trichlorethylene, and alcohol.

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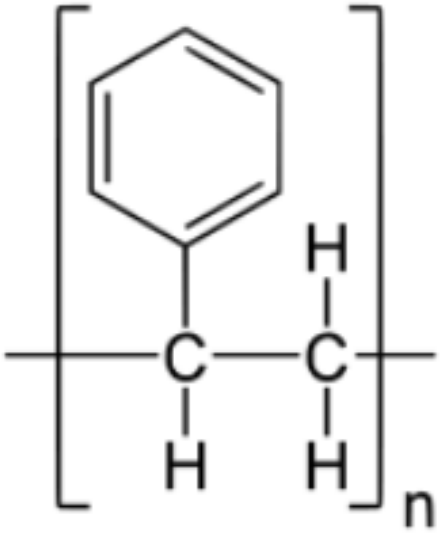

Figure 1: Polystyrene

The strength of the bonds and the mass of the atoms became dependable of the vibration's frequencies. The low Raman shifts has weak bonds and heavy atoms. The high Raman shifts has strong bonds and light atoms. The low- frequencies of carbon-carbon (C-C) interactions are 800 cm-1 on the polyurethane range, whereas high wavelength carbon-hydrogen (C-H) energies are approximately 3000 cm-1. Compared to C-H sound waves C-C vibration feature a more modest intensity. The fact that helium is light in oxygen is the major reason behind this. Two carbon atoms joined by a stronger single bond (C-C) vibrate at around 800 cm-1 whereas several carbon atoms bonded by two stronger bonds (C=C) vibrate in the range of 1600 cm-1. The polystyrene's C-H vibrates may be seen in two areas on the electromagnetic waves, one roughly at 2900 cm-1 and the other at more above 3000 cm-1. In the first instance, the electrons in the carbon atoms become an essential component of carbon chains (also known as "aliphatic"), but in the second one, they are a part of carbon ring structure (also known as "aromatic"). Now you'll find the powerful band at around 1000 cm-1 caused by the phenol ring's expansion/contraction vibrating motions.

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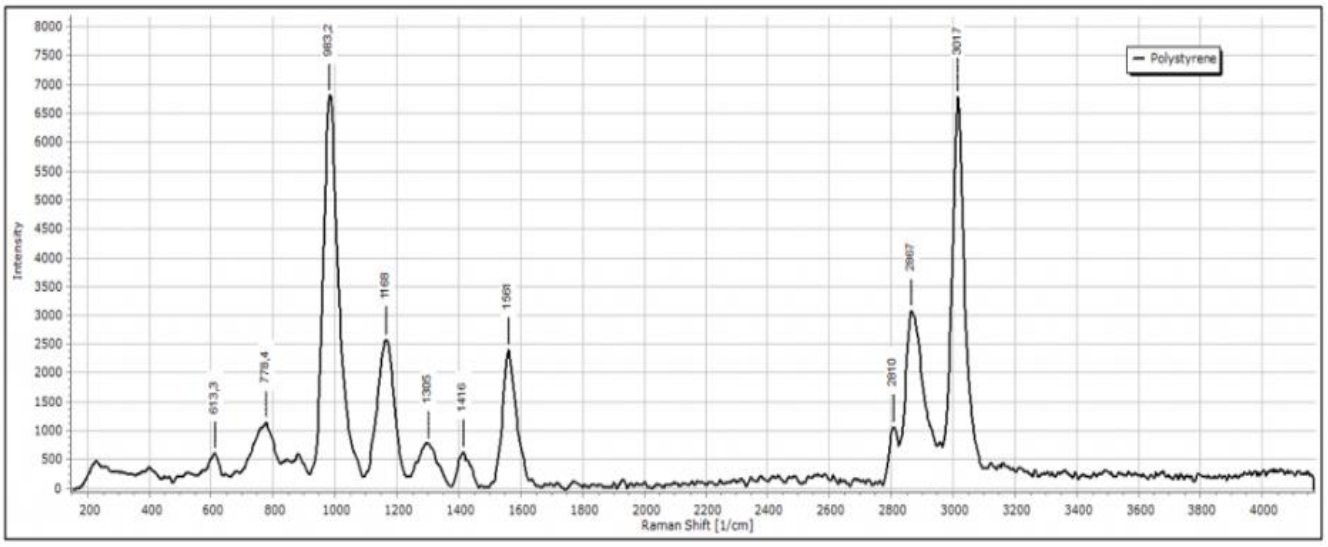

Figure 2: (a) Raman Spectrum of Polystyrene

3.2. Polycarbonate (PC):

A thermoplastic polymer made from acidic substances is called polycarbonate (PC). The type that is made from bisphenol A, whose structural formula is shown in the graphic below, is the most significant.

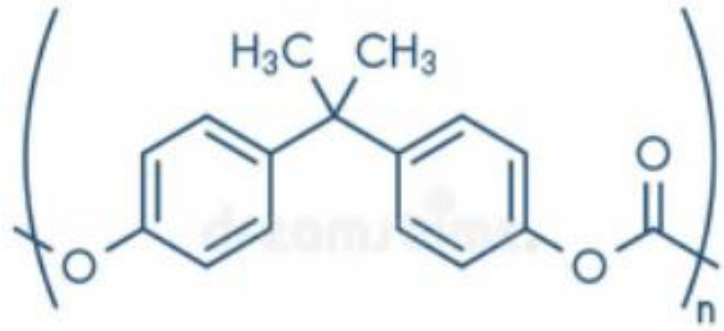

Figure 3: Polycarbonate

The C-C, C=C, and CH3 regions' primary bands are discernible, and the spectrum resembles that of plastic. It varies unlike the last one, especially across the "low" half of the band as well as throughout the band at roughly 3000 cm-1..

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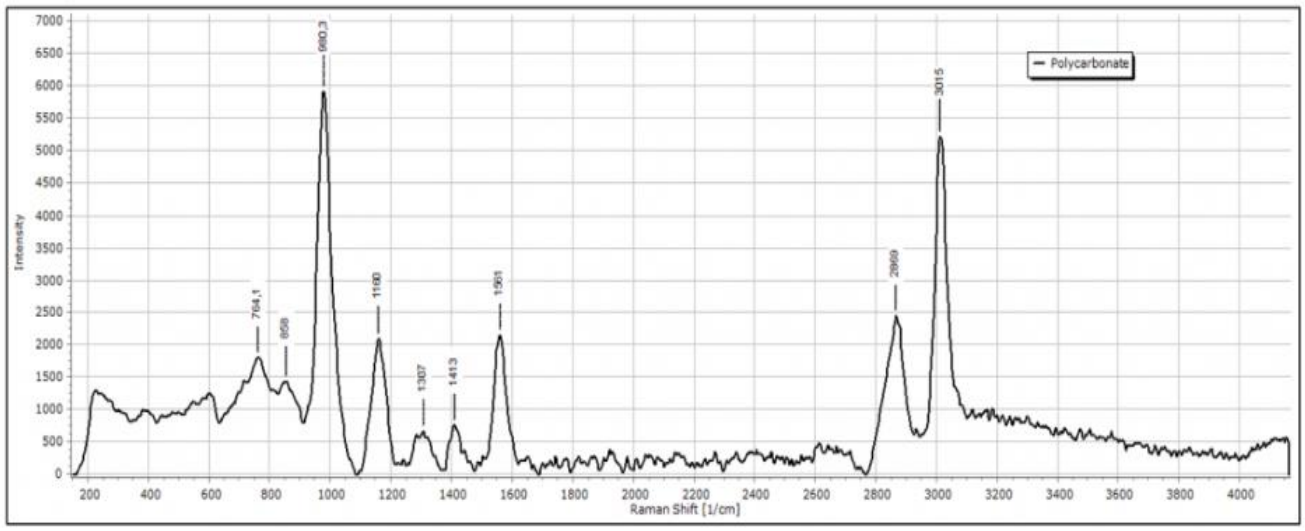

Figure 4 (a): Raman spectrum of Polycarbonate

3.3 Polymethylmethacrylate (PMMA):

The malleable substance Polymethylmethacrylate, also known as PMMA, is made of filaments of methyl methacrylate, or methyl methacrylate, which is an ester of methacrylic acid's methyl ester and is displayed in the picture on its opposite side. A kind of thermoplastic polymers, such as that is. Plexiglas, Perspex and Since are some of its other brand names. It is typically more visible than crystal and has the attribute of being practically indestructible. Its brightness is comparable to the transparent nature of optics fiber..

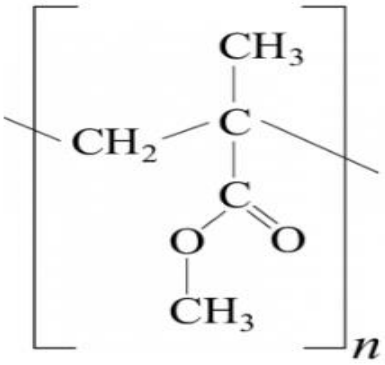

Figure 5: Polymethylmethacrylate (PMMA)

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"The Raman spectrum of PMMA, the main bands due to the C-C, C=C, CH_3 and C-O bonds are recognized."

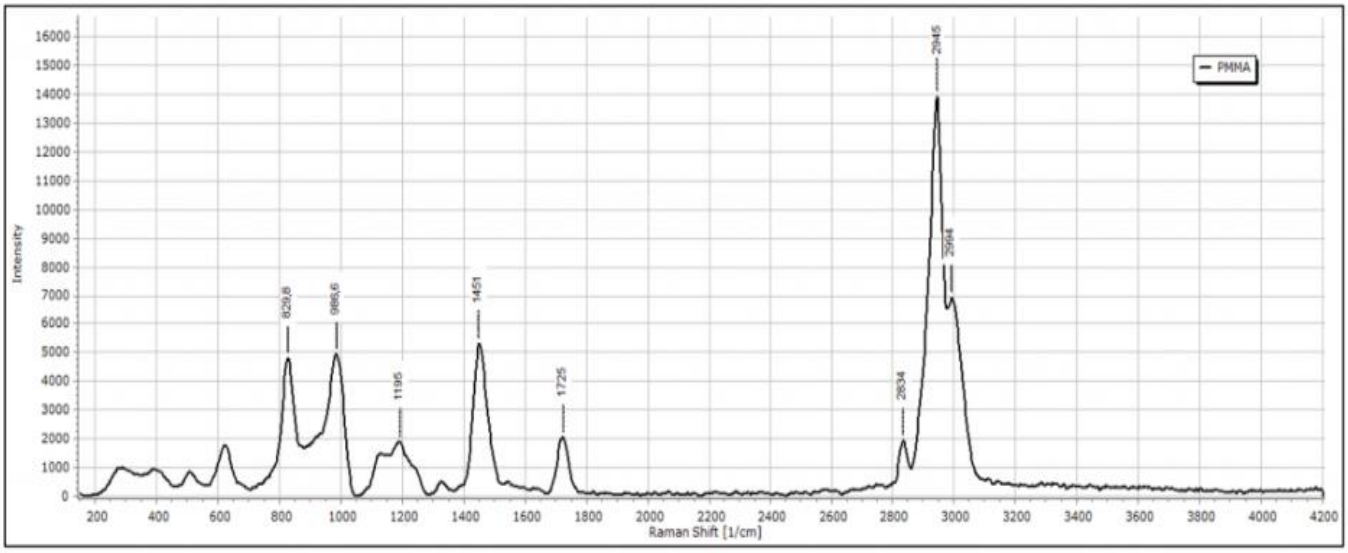

Figure 6 (a): Raman Spectrum of Polymethylmethacrylate (PMMA)

3.4. Polyethylene (PE):

It is quite typical of polyethylene and is the most fundamental of manufactured polysaccharides; it is often referred to as polyamide. It has the molecular formula (-C2H4-)n, and it can polymerize to only a few hundred different levels. The total length and degree of branching of the links might vary. A warm-plastic resin that offers excellent shielding qualities and stable chemistry, polypropylene is a member of the least expensive polymers and may be found in both transparent (amorphous form) along with white (crystalline formed) solid shapes.

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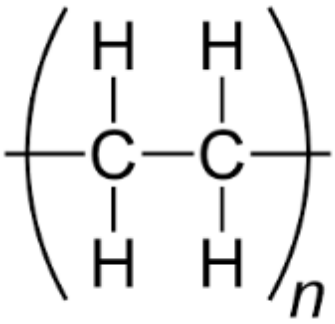

Figure 7: Polyethylene (PE)

The spectrum of Raman rays is presented by the following figure, with the areas caused by C-H bond extending energies at approximately 3000 cm-1, C-H bond rotating and bending energies at 1300 around 1400 cm-1, plus C-C bond extending energies at 1000–1200 cm-1.

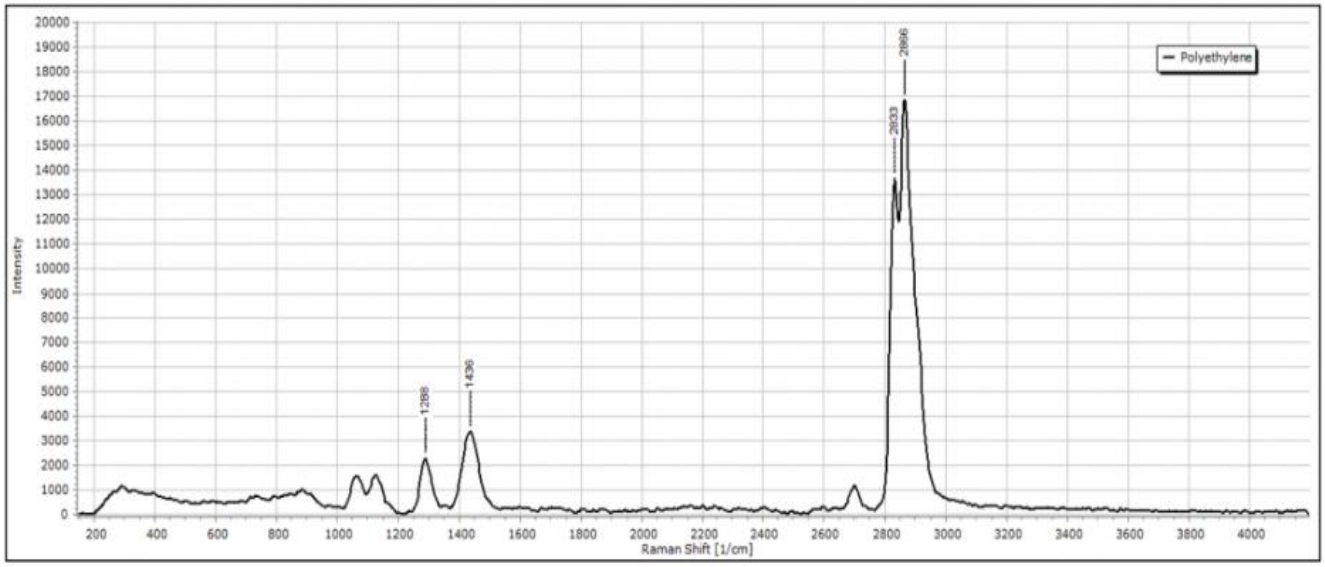

Figure 8(a): Raman Spectra of Polyethylene (PE)

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5. Conclusion

The proposed analyses of the research work discuss the interpretation of the observed data set following the experimental procedure. The consequences of the Raman lines with structural analysis of composition levels was tabulated and results was validated with the source data. The approximation and standard deviation analysis for the quantified data was calculated following the previous analysis and the research outcomes was concluded. This research work discussed different types of Raman spectroscopies in pharmaceutical areas and other areas. Here, different types of polymers and crystal forms such as Polystyrene (PS), polycarbonate (PC), Polymethylmethacrylate (PMMA), "Polyethylene (PE), Polyethylene terephthalate (PET), Polypropylene (PP)", were discussed with their advantages and disadvantages. Polymorphs are very important in pharmaceutical manufacturing because they determine physiological dissolution rates and their control is therefore often critical. This is a quantitative analysis research work where different experimental procedures of Raman spectroscopy have been discussed.

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