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Advances in Applied Science Research, 2011, 2 (1): 125-128

ISSN: 0976-8610
CODEN (USA): AASRFC

FTIR Investigation of Structural Change in Bio-molecule

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ABSTRACT

Infrared absorption spectrum of Biomolecules of gum Arabica is analyzed from measured data of FTIR spectra. The change in characteristics bond vibration detected clearly. The obtained shift of the characteristics frequency caused due to change molecular structure introduced by polymerization effect. The novel technique is important in bio-molecular analysis.

Keywords: Infrared Spectroscopy, Bio Polymer, Gum *Arabica*, Vibrational levels.
PACS: R36.20.Ng; 82.35.Pq; 87.15.rp; 87.15.K-

INTRODUCTION

The study of bio-molecules/ biomaterials are belongs to a high priority open field of research in the recent time. Investigation of internal motion/ dynamics of bio-molecules/ biomaterials are emerging as a new field of research towards (i) Understanding of physics of complex system (ii) internal mechanism of a living system (iii) Development of clean and cost efficient technologies in various field Fourier transform infrared (FTIR) spectroscopy is an emerging analytical tool capable of monitoring IR spectrum of a bio-molecule and hence chemical information, with high signal-to-noise at high spatial resolutions. In an n-atom non linear molecule there are 3n-6 possible vibrational modes. The vibration includes bond bending and bond stretching. The energy difference between vibrational states corresponds to the energy level of IR Radiation. Normally two major region in the IR spectrum of a molecule are the functional group region (7000 Cm -1 to 1500 Cm -1) it includes the X-H stretching region and finger print region (1500 Cm -1 to 350 Cm -1) . The later region is very important in bio-molecular dynamics [1] and it may provide much relevant information about the internal motion of the molecule and is related bio-molecular function in living systems. The objectives of the FTIR spectroscopic [2] study are (i) to recognize the most reliable absorption frequencies for a particular functional group of a bio-molecule (ii) to use the group frequencies to distinguish the spectra of the sample (iii) to understand the factor which complicate (e.g. overtone and combinational bands, Fermi resonance and most important for a bio-molecule – hydrogen bonded system) IR spectra and be able to

recognize the effect that these have on the spectra. In this present work vibrational characteristics of gum Arabica [3] along with its change due to in growing polymerization effect are studied. The gum Arabica is a bio-molecule with polysaccharide in nature. He objective of this paper is the development of an over dynamical characterization of bio-molecules under the purview of this work.

MATERIALS AND METHODS

Sample Preparation

The gum *Arabica* powder specimen (S1) was collected from Merk (India) and was subjected to a sol–gel process along with pure water so that the polysaccharide host chain can form more complex higher polymers over that in normal powder form. The sol specimens are extracted at initial state, 30, 60 and 120 minutes after that. The experimental specimens (S2, S3, S4 and S5 respectively) were developed by adequate drying of the sols at environmental condition.

Experiments

The developed gum *Arabica* specimens (S2- S5) are supposed to exhibit change in molecular structure over that in S1 due prolongation of sol gel process. FTIR analysis on pure gum *Arabica* was carried out to examine its molecular structure and dynamical information. The analysis was carried out using FTIR Model, IR Affinity 1, Shimadzu, Japan, at high resolution using KBr window.

RESULTS AND DISCUSSION

Figure 1 shows the FTIR spectrum gum Arabica specimen between wave number 350 to 4000 cm-1. Broad peaks are obtained in the IR spectrum of gum Arabica at 3365.2 cm-1 (O-H stretching of carbohydrates), 2939.1 cm-1 (CH2 asymmetric stretching), 1379.3cm-1 (CH, CH2 and OH in-plane bending in carbohydrates), 1042.9 cm-1 (C-O stretching region as complex bands, resulting from C-O and C-O-C stretching vibrations), 704.8 cm-1, 641.7 cm-1 and 603 cm-1 (pyranose rings)It shows the distinctive absorption in finger print region at 603 , 641.7 and 704.8 cm-1. The three frequencies represent the characteristics of bond stretching vibration of the bio-molecule.

Figure 2 and Fig.3 show the comparison of the FTIR spectrum of different gum Arabica specimens between wave number 600 to 607 cm-1 and 638 to 645 cm-1 respectively. Figure 2 shows that the characteristics vibration at 603cm-1 decreases while passing from S1 to S5 whereas Fig.3 represents the same corresponding to absorption peak at 641.7 cm-1.

Table I summarizes the mentioned change in absorption frequency at 704.8cm-1. The overall results give a clear picture for change in molecular structure in the bio-molecule due to polymerization.

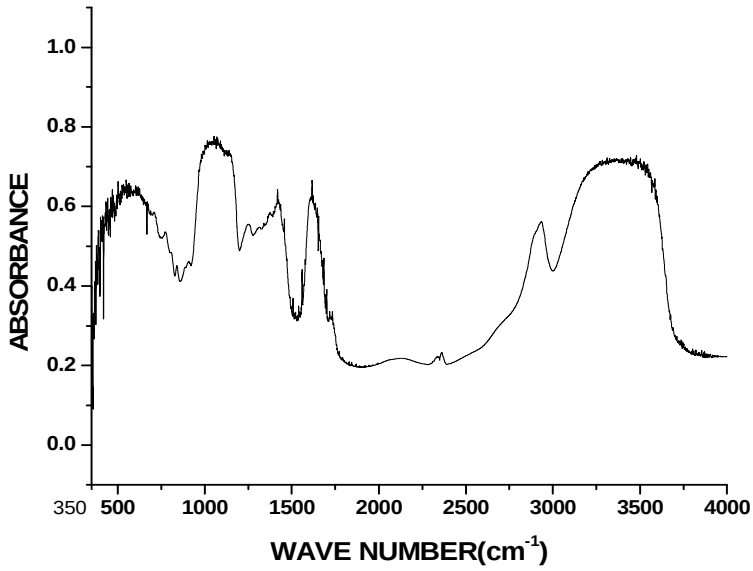

FIGURE 1: FTIR spectrum of sample 1

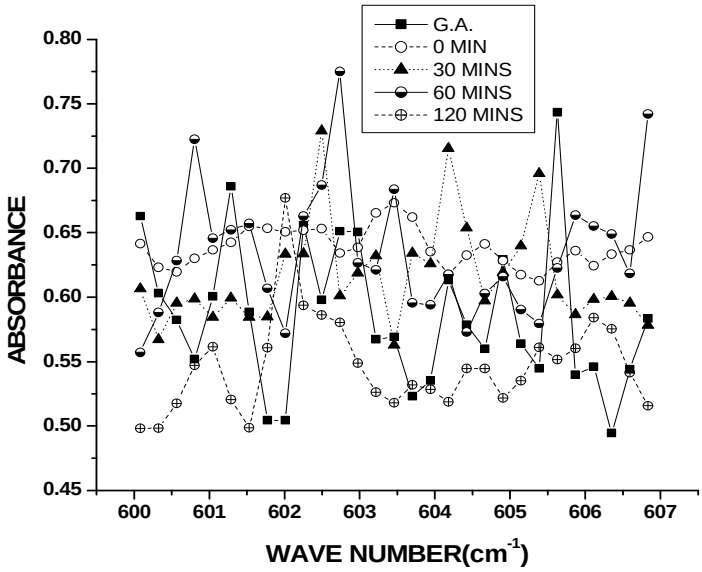

FIGURE 2: FTIR spectrum in between 600 to 607 cm-1

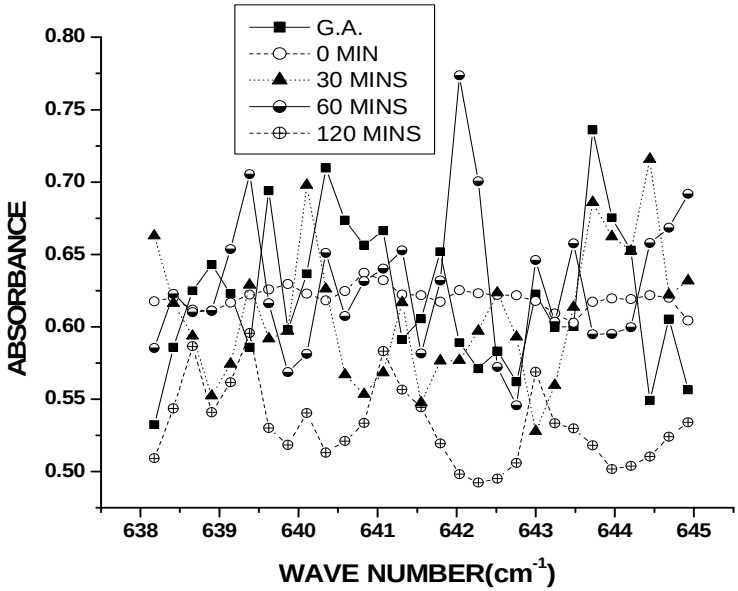

FIGURE 3: FTIR spectrum in between 638 to 645 cm-1

TABLE 1. Comparison of the FTIR spectrum peak for S1 – S5 around wave number 704.8

Wave Number	G.A. (Absorbance)	0 Min (Absorbance)	30 Mins (Absorbance)	60 Mins (Absorbance)	120 Mins (Absorbance)
704.47749	0.59586	0.5822	0.66863	0.59402	0.50622
704.71858	0.6251	0.58692	0.65667	0.64203	0.51766
704.95967	0.61138	0.58325	0.72432	0.66985	0.51106
705.20077	0.81885	0.58042	0.66517	0.64703	0.50187
705.44186	0.59711	0.58188	0.59367	0.75077	0.4769

CONCLUSION

The change in molecular structure, of the constituent bio-molecules of gum Arabica, due polymerization is directly determined from analysis of FTIR spectrum in finger print region. This novel technique may be applied to bio-molecular analysis.

Acknowledgments
Authors Arup Dutta and A.Sarkar are thankful to UGC, New Delhi for the support MRP No f.35-7/2008(SR).

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