ABSTRACT

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Title: - "Investigation of low lying energy levels of internal motion in Bio-molecules and their complexes by Mid & Far FTIR Spectroscopy"

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The work presented in this thesis aiming to the title of it. Biomolecules are molecules that occur naturally in living organisms. The basic building block of life and bio-materials are the bio-molecules. The study of bio-molecules is similar to that of atoms, molecules, and solids. The understanding of mentioned simpler systems may help in investigations of the more complex bio-molecules. Some features are alike in these quantum-mechanical systems; ideas and concepts from molecular and condensed matter physics can thus be taken over directly. Progress in physics has often followed a path in which three areas are essential namely, structure, energy levels, and dynamics. (Structural analysis techniques have progressed and the latest breakthroughs due to Infra red (IR) which allow numerous structure-function studies, particularly the quantitative identification of the atomic assembly of large bio-molecules and the determination of the microstructure of biological tissue in dynamic situations.). Since the subject is vast only overview of the mentioned aspects are given.

The molecular spectroscopy is one of the important investigation tool used in this research however a brief discussion of its methodology is heighted here. When the intensity of the IR source is the extremely bright light provided by a synchrotron or with FTIR spectrophotometer with high signal to noise ratio, it is possible to obtain an excellent IR spectrum. The technique may be comparable to non-destructive testing in Physical/ Material Science/Life Science. In this research scheme the following studies are carried out (i) Investigation and extraction of internal motion from IR spectrum of bio-molecules/ biomaterials, (ii) Development of understanding on internal motion of complex system, (iii) Observation of the functional behavior of bio-molecules from the variation of IR spectrum and dielectric Spectrum with variation of (a) external factor (b) environmental variation (c) introduction of defects. (iv) Preparation of a comprehensive analysis on internal motion and relaxation mechanism of

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biomolecules as complex system. (v) Development of an over dynamical characterization and quantum energy level map of bio-molecules are performed.

The analysis of the results obtained involve type of absorption spectroscopy depending upon the frequency range of the electromagnetic radiation absorbed *Microwave spectroscopy* involves a transition from one molecular *rotational energy level* to another. Molecules may undergo several types of motion. - *translational motion, rotational motion about its internal axes*, and *the vibrational motion.* The absorption in the far infrared corresponds to transitions from an initial state to a low energy final excited state. For isolated molecules, this excitation corresponds to rotational transitions, vibrational excitations of large molecules or roto-vibrational transitions. Their measurements at high resolution provide a better description and understanding of species or chemical reaction.

During this research program few standard bio-molecular system (whose structural and chemical characterization are available or Computer Molecular Dynamical Simulation data may developed or available) are investigated in details and compared with appropriate CMD results. In this research work an adequate analysis of the spectroscopic (FTIR) results are undertaken. The bio-molecular functions of the same system under external factors (temperature, hydration, etc) are investigated in details. Following the results a range of bio-molecular system (e.g. Acacia Arabica, Gum Agar, Manitol Sugar, human hair etc.) are investigated and analyzed. In the last part of this research program some of the mentioned bio-molecule are investigated and analyzed from quantum theoretical simulation. This research project likes to devise a technique for characterization of bio-molecules and more about this subject. The said characterization is expected to be an important outcome from the results of the study of Mid-Far IR (FTIR) of native and modified bio-molecules. The characteristics differences in vibrational/ rotational spectra of modified bio-molecules over the corresponding pure one will provide a possible roadway to characterize defect bio-molecules. The outcome of this research is good, concise and believed to provide a quantum energy map for the low lying states.

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