STUDY OF STRUCTURE, DYNAMICS AND ELECTRONIC PROPERTIES CONDUCTING POLYMERS USING QUANTUM CHEMICAL CALCULATIONS

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ABSTRACT

For a successful molecular design of conducting polymer it is very important to have a complete understanding of relationship between the chemical structure of the polymer and its electronic properties such as its ionization potential, electron affinity and bandgap because polymeric materials are greatly influenced by their macromolecular conformation. Although conducting polymers have received considerable attention, there is still much to be learned about their structure and propertries. Vibrational spectroscopy in conjugation with quantum chemical calculations has always proven to be useful in gaining insight into the electronic properties of conjugated polymers. One approach to understand the behaviour of complex, polymeric materials is to prepare and study oligomeric analogues. Therefore, structural and spectral characteristics of polydibenzofulvene (PDBF) have been studied by vibrational spectroscopy and quantum chemical methods. Electrostatic potential surface, optimized geometry, harmonic vibrational frequencies, infrared intensities and activities of Raman scattering were calculated by density functional theory (DFT) using oligomeric approach. A complete analysis of the observed infrared and Raman spectra has been reported on the basis of wavenumber of vibrational bands and potential energy distribution. The infrared (shown in figure) and Raman spectra of the molecule based on DFT calculations show reasonable agreement with the experimental results.

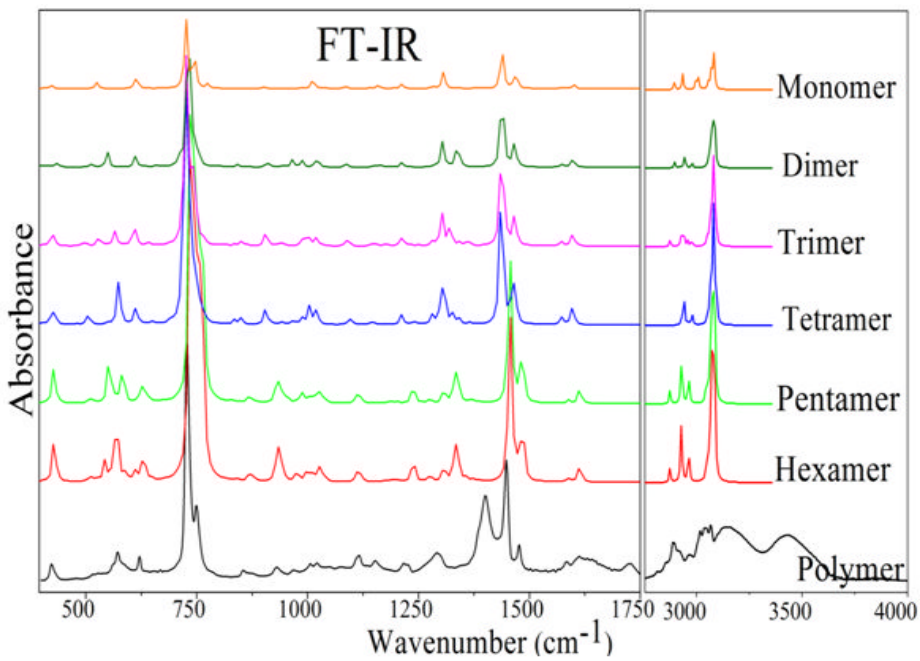

Figure. Experimental and calculated (scaled) FT-IR spectra of PDBF.