Visualizing a Cycloaddition by the Abinitio SCF Methods for the Formation of Polystyrene, a Polymeric Material

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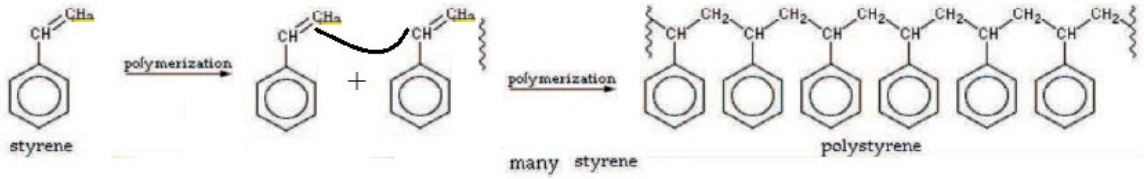
There have been several sources from where adequate knowledge can come forth on the formalisms developed based on Quantum Mechanics and Molecular Mechanics for the Calculation of Molecular Properties. Isolated molecules mostly predominate for the systems subjected to such calculations. When it is a question of ensemble of molecules to be subject of study, then several ways have been found to put to use these formalisms with appropriate modifications to handle the inter molecular interactions to consolidate the ensemble properties relatable to the individual molecule properties in which case only the intra molecular properties are important. The ensemble of molecules could be in any of the well known states of matter namely Solid, Liquid and Gas.

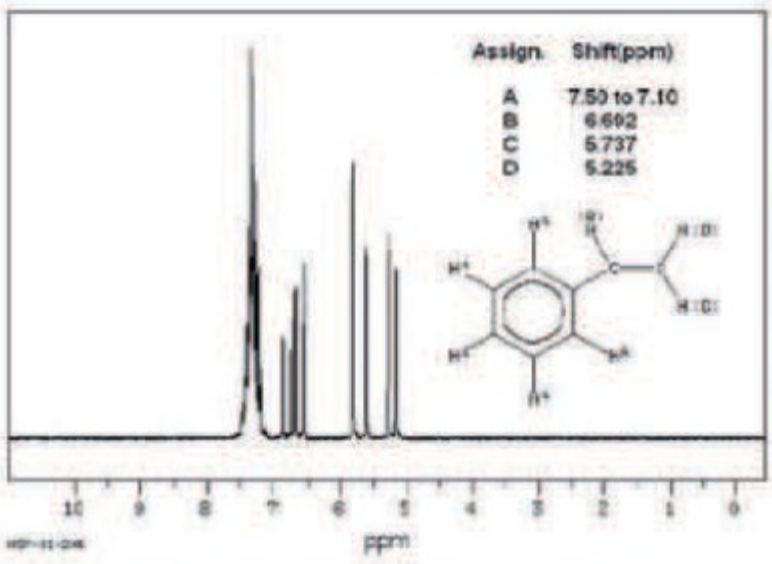
It is not intended to describe the above aspects much in this lecture. The main description would be about how already known soft ware can be put to effective
calculations that give explanations in reconciling with experimental findings which were not simple enough to interpret. In such theoretical methodology, it is not simply the Molecular Orbital calculations which were computationally relevant but also modelling the system and verifying the model by simulations further consolidation by the QM methods for isolated molecules and ensembles are adapted. In this context properties of materials are an important aspect which is becoming potentially the subject several investigators are engaged in. "Applications to materials" has a wide scope from the point of view of the utility of the Quantum Mechanics based methodology.

One of the important classes of materials is the Polymers. The structure of these polymeric substances determines such physical properties like texture and morphology, and also the stability, durability and longevity of their utility. One such case is the styrene polymer. This case to be described in this lecture involves several considerations which are not a matter of routine application of calculation soft ware but requires a ingenuity to adapt several methods to suit to evidence the experimental facts. The case to be considered in this lecture would be mainly a question of explaining a spectroscopic finding: the spectral pattern, interpretations, and the insight into possibly the reality about the material structure.

An e-flipbook is available online at URL: http://anyflip.com/ddoa/jydw/

In the following sheet, a few figures from the book is copied to draw attention and for familiarity at the outset.





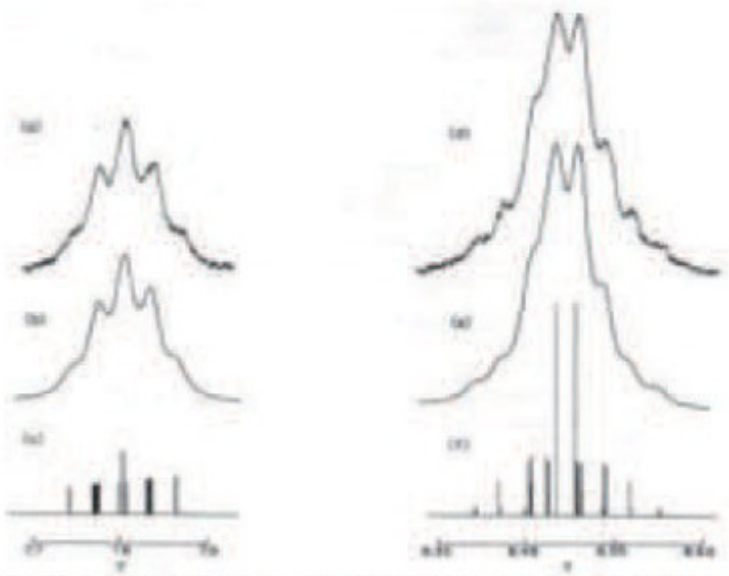


Fig. VI-3. 220 MHz backbone proton spectrum of isotactic polystyrene, 2% in *o*-dichlorobenzene at 130°. (a) and (d) are the experimental spectra of the α- and β-protons, respectively; (b) and (e) are spectra calculated with the parameters shown in Table VI-1 (for 130°); (c) and (f) are "stick" spectra corresponding to (b) and (e) (Heatley and Bovey[7]).