"Spectroscopic Studies of Buckminsterfullerenes"

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The electronic absorption spectra of C_{60} and C_{70} molecules are recorded in different phases, viz. solution, sol-gel, polymer and thin film using Jasco UV/ VIS/NIR Spectrophotometer (Model V-570). In solution form the polar, aliphatic and aromatic solvents have been used, which show the spectral red shift from polar to aliphatic and from aliphatic to aromatic. The glass form fullerenes have been prepared using the sol-gel technique. For the polymer film, the fullerene C_{60}/C_{70} was dissolved in toluene and polystyrene in the ratio 9:1. Thin films of C_{60} and C_{70} were deposited on the glass substrate by vacuum evaporation technique using vacuum coating unit (Model EYU-3000S, VEQCO) keeping the substrate at room temperature and in vacuum of 10^{-5} torr. The electronic absorption spectra in these matrices are compared.

To understand the characteristics of the electronic state and structure of three dimensional C_{60} and C_{70} molecules, *Zerner's Intermediate Neglect of Differential Overlap* (ZINDO) method has been used. The ground state molecular structures of the fullerenes are fully optimized using ZINDO/1 (CI) method and compared with the available experimental as well as other reported theoretical data. The calculated geometrical parameters for C_{60} molecule are found in which HOMO-LUMO gap is 5.49 eV, bond lengths are R(5-6) 1.451 Å and R(6-6) 1.397 Å and first ionization potential is 6.55 eV. After geometrical optimization of C_{70} molecular structure, the HOMO-LUMO gap is found as 4.8 eV and bond lengths are 1.43 Å and 1.46 Å. These fully optimized geometries of C_{60} and C_{70} molecules are further used for the ZINDO/S calculations to find out the electronic transitions. The main aim was the interpretation of the electronic spectra of C_{60} and C_{70} molecules that have been studied experimentally as well as theoretically. The ZINDO/S calculation predicts the electronic transition energies and oscillator strength for every weak, medium and strong band. For these molecular orbital calculations of fullerenes C_{60} and $C_{70,}$ Hyperchem 5.0 software has been used which was obtained from Hypercube, Inc. USA.

On the other hand, the emission bands for C_{60} and C_{70} molecules in non-polar solvents (aromatic) are investigated using the classical Aminco-Bowman spectrophotometer with Xenon lamp to record a particular emission band for a particular electronic absorption band and laser induced fluorescence (LIF) set-up used to record the fluorescence spectra with Nitrogen laser at 337.1 nm wavelength as excitation source for both the fullerene molecules. The spectral difference in the fluorescence spectra obtained using different

sources, which is due to the sensitivity of the set-up. The classical spectroscopy has lower sensitivity so that the spectral bands are broader than that of the laser induced spectral bands.

Moreover the FTIR spectra for C_{60} and C_{70} molecules are recorded using Fourier Transform Spectrophotometer RX - 1 model of Perkin Elmer (U. K.) with 400-4000 cm^{-1} range, to find out the IR frequencies and transmittance. The samples were prepared in nujol using the mulling process for both the molecules. From the FTIR Spectra it is predicted that the C_{70} molecule has less symmetry as it has many vibrational modes as compared to C_{60} molecule, which is highly symmetric.