

338. Spectroscopy in UV-VIS and IR Region in Different Environment

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Abstract. Photophysical process is ubiquitous in nature, playing a key role in the light harvesting machinery of photosynthesis, where hundreds of special antennae molecules are used to collect light and transfer the absorbed energy towards reaction centers where charge separation occurs. This work is an effort to explain the study of environment effects on the energy transfer. The study has its special interest on the use of different spectroscopic tools working in UV-VIS and IR region to identify intra/intermolecular charge transfer photophysics of different compounds which are active DNA bases which will be easily understandable to all.

Introduction

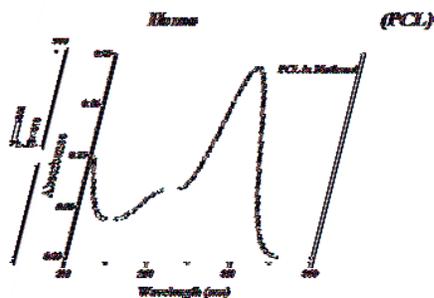
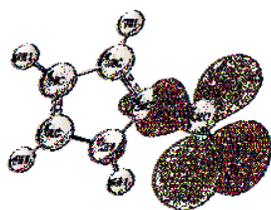
Among different hydrogen bonds, the O-H...O and N-H...O bonds most often occur in liquid phase. It plays a crucial role in biological systems such as proteins and DNA base pairs and is essential for life processes. In all hydrogen bonded molecules there is a strong possibility of solute and solvent interaction. There is a lot of studies deal with these interactions to explain their nature, strength and other features important for physical, chemical, and biological processes such as proton transfer reaction, molecular association in solutions etc. Proton transfer spectroscopy ground and excited state reaction dynamics of N-heterocyclic [1,2] is an interesting and developing subject area of research especially for the molecules containing more than one functional group.

Methods

Absorption and emission spectrum in mid IR and uv-vis region reflects features of all molecules as a whole. This fact suggests that the coupling of *ab initio* calculations [3] of vibrational modes and mid-IR spectroscopic measurements may be another powerful tool for studying the structural properties of Pyrrole-2-Carboxylaldehyde (PCL), Pyrrole-2-Carboxylic acid and its related compounds. The intramolecular redistribution of electronic charge due to photonic excitation induces the ESIPT process which is ultrafast in nature [4].

Results & Discussion

The absorption spectra of PCA in different solvent point the presence of intramolecularly hydrogen bonded closed conformer in the form of 280 nm band. Stokes shifted fluorescence of PCA at 310 nm in hydrocarbon solvent and hydroxylic solvents have been identified to be due to normal molecule. Variation of pH results enhancement or decrease of emission from ionic conformer with parallel dwindling of emission of neutral species. Theoretical and experimental ground state and excited state behavior of PCL and its related compounds were investigated in UV-VIS and mid IR region of electromagnetic spectrum. We have measured the spectrum of PCL in the UV-VIS region ranging from 190 nm to 900 nm and in IR region ranging from 450 cm^{-1} to 4400 cm^{-1} . Possible origins of dominant absorption bands have been assigned successfully with *ab initio* HF and DFT calculations taking the effects of hydrogen bonds in account in the IR region. Possibility of intramolecular and intermolecular hydrogen bonding of PCL in ground state was established theoretically by the distance N5-H6.....O11 of acidic and basic moieties of PCL and experimentally it is verified by the IR stretching and bending mode vibrations of different parts of the molecule [5]. The possibility of transfer of hydrogen from pyrrole ring towards formyl ring in excited state indicates in the light of difference in bond length and bond angle, dipole moment, enthalpy, Gibbs free energy etc and with fluorescence and phosphorescence spectrum in the excited state of the molecule. The absorption maximum and oscillator strength computed from HF (RHF, UHF), DFT calculations for gas phase, nonpolar medium, polar medium agrees reasonably well with experimentally measured data. We consider that the experimental and theoretical results presented here are useful for studying the electronic and vibrational properties of different olefins.



UV-VIS absorption spectra of PCL in MeOH.



IR absorption spectra of PCL in KBr pellets.

References

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