AB INITIO AND DFT STUDIES ON THE SPECTROSCOPY AND PHOTOPHYSICS OF ANTHRANILIC AND SALICYLIC ACIDS

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Ab initio and DFT calculations have been carried out at Hartee-Fock (HF) and B3LYP level using different basis sets to study the IR spectra of monomers and dimmers of Anthralic and Salicylic acids. The excited state energies were determined to explore the photophysical properties of these systems, using Time Dependent DFT calculations along with CIS calculations. A comparison of the hydrogen bonding properties of Salcylic acid and Anthranilic acid shows both similarities and differences between the two molecules. The ab initio potential energy profile for the rotamarisation in the each molecule were derived. Studies on the spectroscopy and photophysical properties of these two molecules are summarized and compared.[a] The phenolic OH stretching vibration in the Salicylic acid monomer shifted towards the low wavenumber side upon electronic excitation due to hydrogen atom dislocation. Further work is presently in progress.

[a] C. A. Southern, D. H. Levy, G. M. Florio, A. Longarte, and T. S. Zwier; J. Phys. Chem. A, 107, 4032 (2003)