

Photophysics and photochemistry of Indole and Indole derivatives : A quantum chemical study

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Indole, being the main chromophore of amino acid tryptophan and several other biologically relevant molecules e.g. serotonin, melatonin etc., has prompted considerable theoretical and experimental interest. Indole and indole derivatives also act as fluorescence marker in biological systems. One important property of indole chromophore is its sensitivity to the environment. The excited state dynamics of indole is challenging due to simultaneous involvement of several vibrational modes. Our work focuses on the investigation of photophysical and photochemical properties of indole by means of theoretical and computational methodologies. Having three close-lying excited electronic states, the vibronic coupling effect becomes extremely important in the photophysics and photochemistry of indole. The effect of ring substitution on the photophysical properties of indole is explored for several indole derivatives of biological importance. Vibrational analysis is carried out to identify important modes contributing to photodynamics. One-dimensional excited state potential energy cuts are calculated along the important vibrational modes using time-dependent density functional theory methods. The vibronic model Hamiltonian is parametrized by the fitting of potential energy function with the *ab initio* data for the purpose of exploring the time-scale and mechanism of excited state dynamics.

References:

1. P. Mondal et al., J. Photochem. Photobiol. A (2020), **387**, 112164.
2. A. L. Sobolowski and W. Domcke, Chem. Phys. Lett. (1999), **315**, 293.
3. C. Brandt et al., Phys. Chem. Chem. Phys., (2010) **12**, 4968.