A THEORETICAL STUDY OF SUBSTITUENT EFFECTS ON THE EXCITATION ENERGIES OF 2-PYRIMIDINONE AND PURINE DERIVATIVES

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Being able to predict and tune the absorption and fluorescence properties of chromophores is important especially in designing fluorescent probes or dyes. Electronic structure methods enable us to study these properties by calculating excited electronic states and their potential energy surfaces. To probe how excitation energies and photophysical behavior relate to molecular structure, we have calculated substituent effects on the vertical excitation energies and potential energy surfaces for a number of derivatives of 2-pyrimidinone and purine bases. Correlations between the molecular structure and the photophysical behavior can be made based on these results, which may be used as tools for future attempts to design molecules with the desired absorption and fluorescence behavior.