Characterization of Excited States via FFT Time-correlation functions: IR spectrum for Conjugated Molecules

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Abstract

Energy transfer is critical in many aspects of life. It is crucial in photosynthesis, as well as in the development of new technological devices such as biosensors, photovoltaics and light emitting devices. Therefore, characterization of conjugated molecules' excited states has become an important issue. We have studied a family of two- and three- ring linear poly(phenylene ethynylene) dendrimers that mimic the storage and energy transport that occurs in photosynthetic systems. We performed IR spectroscopy calculations using linear response theory and we analyzed the propagation of some ground state normal modes in the excited states. Our results show the difference between two isomers, where one of them looks like a good candidate for energy transfer process. We also show that IR spectroscopy can be applied to the characterization of the different states of these molecules.

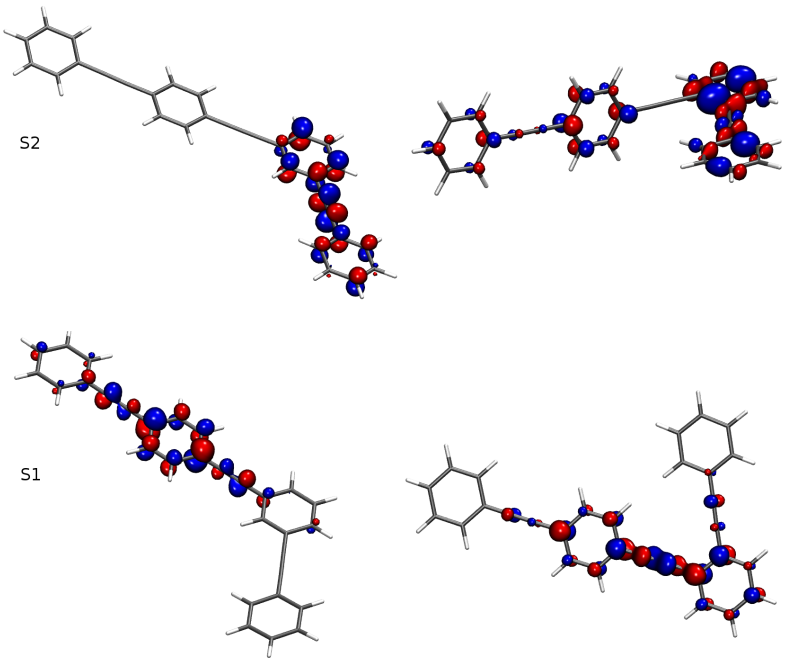

Figure 1: Transition density matrix representation for the first two excited states (S1 and S2) of the meta- and ortho-conjugated systems.