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The effect of structural conformations and solvent effects in a light-harvesting Carotenoid-diaryl-Porphyrin-C_{60} (CPC_{60}) molecular triad on the charge transfer excitation energies[1] TUNNA BARUAH, MARCO OLGUIN, RAJENDRA ZOPE, University of Texas at El Paso — We present a detailed study of charge transfer (CT) excited states for a large number of structural conformations in a light-harvesting Carotenoid-diaryl-Porphyrin-C_{60} (CPC_{60}) molecular triad. The molecular triad undergoes a photinduced charge transfer state exhibiting a large excited state dipole moment, making it suitable for application as a molecular-scale optoelectronic device. One important consideration is that the conformational flexibility of the CPC_{60} triad impacts its dynamics in solvents. Since many experimental photochemical measurements for the traid are made in solution, studying the effect of conformational changes on the CT energy furthers the understanding of its photoconversion properties. We have calculated a few low lying CT excited state energies for a series of triad conformers, where the conformers were generated by incrementally scanning a 360 degree torsional (dihedral) twist at the C_{60}-porhyrin linkage and the porphyrin-cartotenoid linkage. The CT excitation energy was calculated at each 45 degree dihedral increment. Addtionally, several different CPC_{60} conformations were taken from molecular dynamics simulations of the triad in water and other solvents of varying polarity. Our calculations show that structural change

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Tunna Baruah
University of Texas at El Paso

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