

Abstract Submitted
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Effect of geometrical orientation on the charge transfer energetics of supramolecular (tetraphenyl)-porphyrin/fullerens dyads¹ MARCO OLGUIN, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — We present our study of several low lying charge-transfer (CT) excitation energies for a widely used donor-acceptor system composed of a porphyrin-fullerene pair. The dyad systems consist of C₆₀ and C₇₀ acceptor systems coupled to tetraphenylporphyrin (TPP) and tetraphenyl-(zinc)porphyrin (ZnTPP) donor systems in a co-facial orientation. We find that replacing C₆₀ by C₇₀ in a given dyad may increase the lowest charge transfer excitation energy by about 0.27 eV, whereas varying the donor in these complexes had marginal effect on the lowest charge transfer excitation energy. Additionally, we examined the effect of geometrical orientation on the CT energy by calculating several CT excited state energies for an end-on orientation of the porphyrin-fullerene dyads. The CT excitation energies are larger for the end-on orientation in comparison to the co-facial orientation by 0.6 eV - 0.75 eV. The difference is attributed to a reduced exciton binding energy in going from the co-facial to the end-on orientation.

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