

Abstract Submitted
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Electronic structure and charge transfer states of a multichromophoric heptad¹ LUIS BASURTO, RAJENDRA ZOPE, TUNNA BARUAH, University of Texas at El Paso — A multichromophoric Heptad molecule containing Zn-tetraphenyl porphyrin, BDPY dye, bisphenyl anthracene, and C₆₀ attached to a hexaphenyl -benzene core was synthesized by Gust et al. (J. Phys. Chem. B, 113, 7147 (2009)). The snowflake like molecule behaves like an antenna capturing photons at different wavelengths and transferring the energy to the porphyrin. We present a DFT based study on the ground state of the complex and also on the lowest two charge transfer (CT) states of the complex carried out using a perturbative delta-SCF method. The calculations, done using a mixed all-electron and pseudo-potential approach, show that the ionization potential of porphyrin and the electron affinity of C₆₀ in the complex changes significantly from isolated molecules. Our calculated value of the lowest CT state is within 0.2 eV of the experimental estimate. This CT state contains a hole on porphyrin HOMO and a particle on the C₆₀ LUMO. A comparison of the energetics with experiment indicates that the process probably involves excitation from the HOMO-1 of porphyrin to the porphyrin LUMO followed by electron transfer and hole bubbling up resulting in a CT state with the hole on porphyrin HOMO and particle on C₆₀ LUMO.

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