Artificial Photosynthesis: Porphyrins-Fullerene Molecular Complex

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Fullerene, chemical structures made of C atoms, and especially its C_{60} stable form (60 carbon atoms arranged in a soccer ball-shaped structure [1]) proved to have photo- , electro-chemical and physical properties [2] that can be exploited in many and different biological fields. C_{82} and C_{96} are members of fullerene family reported in 1992 [3]. Besides a wild range of fullerene application in different fields, scientific interest has also been showed on the field of photosynthesis [4]. Photodynamical studies on porphyrin and analogs-fullerene linked systems have been studied [4] and some efficient photo-voltaic cells constructed on semiconductor nanoparticle have been reported [5]. In this context, a new porphyrin-fullerene system is proposed as a new complex able to absorb better the light in the range of wavelengths of visible spectrum and was investigated. In this study, two porphyrins were linked together through a C_{96} fullerene. The structural optimization of the investigated structures was conducted with Spartan '10 *ab initio* package at the restricted (post) Hartree-Fock (HF) level of theory with STO-3G refinement. Two porphyrins were bind to a C_{96} fullerene in such manner to assure a minimum torsion of the bind. Two version of the obtained structure were investigated - with and without an Mg and Fe pair. The usefulness of the Mg-Fe pair has been derived from [6]. Characteristics of the investigated systems are as follow: ① formula: $C_{28}H_{52}N_4$, weight = 444.752 amu, area = 1134.04 $Å^2$, volume = 1731.94 $Å^3$, PSA = 65.508 $Å^2$, ovality = 1.63, E-HOMO = -2.49 eV, E-LUMO = 2.11 eV, dipole moment = 2.55 debye, polarizability = 40.29; ② formula: $C_{152}H_{48}FeMgN8$, weight = 2066.264 amu, area = 1104.75 $Å^2$, volume = 1715.47 $Å^3$, PSA = 23.094 $Å^2$, ovality = 1.59, E-HOMO = -2.68 eV, E-LUMO = 1.90 eV, dipole moment = 2.99 debye, polarizability = 40.29. The first porphyrin-fullerene system showed good absorption in the range of visible spectrum (300-600 nm). Unfortunately, the second one was too huge to perform accurate calculations. The obtained results provide important information and open a gate for the development of photoinitiated molecular devices.

References

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