

Accepted Manuscript

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PII: S0167-7322(18)33532-3
DOI: doi:[10.1016/j.molliq.2018.08.117](https://doi.org/10.1016/j.molliq.2018.08.117)
Reference: MOLLIQ 9562
To appear in: *Journal of Molecular Liquids*
Received date: 9 July 2018
Revised date: 10 August 2018
Accepted date: 21 August 2018

Please cite this article as: Subrata Nayek, Sneha Paul, Ajoy Bauri, Anamika Ray, Sumanta Bhattacharya , Molecular assembly of PC70BM with a designed monoporphyrin: Spectroscopic investigation in solution and theoretical calculations. Molliq (2018), doi:[10.1016/j.molliq.2018.08.117](https://doi.org/10.1016/j.molliq.2018.08.117)

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Molecular assembly of PC₇₀BM with a designed monoporphyrin: Spectroscopic investigation in solution and theoretical calculations

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Abstract

The present paper reports a detailed photophysical investigation on the supramolecular interactions of a functionalised fullerene, namely [6,6]-phenyl C₇₁ butyric acid methyl ester (PC₇₀BM), with a designed monoporphyrin, [bis(4-hydroxyseseliny)porphyrin] (**1**), in toluene and 1,2-dichlorobenzene (DCB). The values of the binding constant (*K*) for the PC₇₀BM-**1** system measured by steady-state fluorescence investigation in toluene (*K*_{PCBM-1} (toluene)) and DCB (*K*_{PCBM-1} (DCB)) are estimated to be 15,085 dm³·mol⁻¹ and 6,700 dm³·mol⁻¹, respectively. A moderate value of selectivity (*K*) is observed for the PC₇₀BM-**1** system in toluene and DCB (*K*_{PC70BM-1} (Toluene)/*K*_{PC70BM-1} (DCB) ~ 2.25) due to a solvophobic effect. Life time measurements proved that photo-excited **1**^{*} undergoes decay in the presence of PC₇₀BM in toluene and DCB as a result of static quenching. Hybrid-density functional theory (DFT) calculations predicted the geometric structure of PC₇₀BM-**1** system *in vacuo* and established the electronic redistribution between PC₇₀BM and **1** in the PC₇₀BM-**1** system with the help of molecular orbital, molecular electrostatic potential map, and multipole bond moment calculations. Transient-absorption measurements established that binding interactions overcome both energy and/or electron-transfer process(es) during non-covalent interactions between PC₇₀BM and **1** in solution.

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