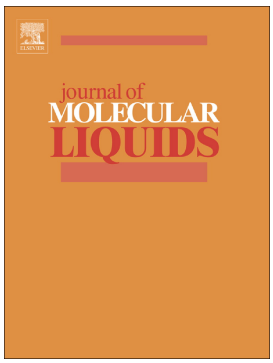

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Molecular assembly of $PC_{70}BM$ with a designed monoporphyrin: Spectroscopic investigation in solution and theoretical calculations

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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 C_{71} butyric acid methyl ester ($PC_{70}BM$), with a designed monoporphyrin, [bis(4-hydroxyseselinyl)porphyrin] (**1**), in toluene and 1,2-dichlorobenzene (DCB). The values of the binding constant (K) for the $PC_{70}BM$-**1** system measured by steady-state fluorescence investigation in toluene ($K_{PCBM\text{-}\mathbf{1}}$ (toluene)) and DCB ($K_{PCBM\text{-}\mathbf{1}}$ (DCB)) are estimated to be 15,085 $dm^3 \cdot mol^{-1}$ and 6,700 $dm^3 \cdot mol^{-1}$, respectively. A moderate value of selectivity (K) is observed for the $PC_{70}BM$-**1** system in toluene and DCB ($K_{PC70BM\text{-}\mathbf{1}\ (Toluene)}/K_{PC70BM\text{-}\mathbf{1}\ (DCB)} \sim 2.25$) due to a solvophobic effect. Life time measurements proved that photo-excited $\mathbf{1}^*$ undergoes decay in the presence of $PC_{70}BM$ in toluene and DCB as a result of static quenching. Hybrid-density functional theory (DFT) calculations predicted the geometric structure of $PC_{70}BM$-**1** system *in vacuo* and established the electronic redistribution between $PC_{70}BM$ and **1** in the $PC_{70}BM$-**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 $PC_{70}BM$ and **1** in solution.