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Anamika Ray, Sumanta Bhattacharya



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Molecular complexation between PCBM and porphyrazine in solution: a case study of non-covalent interaction

Anamika Ray and Sumanta Bhattacharya*

Department of Chemistry, The University of Burdwan, Golapbag, Burdwan – 713 104, India.

Abstract

The present investigations report the non-covalent interaction of a fullerene derivative, namely, [6,6]-phenyl C₇₁ butyric acid methyl ester (PC₇₀BM) with 2,7,12,17-tetra-tert-butyl-5,10,15,20-tetraaza-21H,23H-porphine (**1**) and zinc-2,7,12,17-tetra-tert-butyl-5,10,15,20-tetraaza-21H,23H-porphine (**2**) in toluene and also in mixed solvent comprising toluene and 1,2-dichlorobenzene (volume:volume = 3:2). Complex formation by steady state fluorescence studies reveal high value of binding constant (K) for both PC₇₀BM-**1** and PC₇₀BM-**2** systems in toluene, i.e., $K_{\text{PCBM-1}} = 10,820 \text{ dm}^3 \cdot \text{mol}^{-1}$ and $K_{\text{PCBM-2}} = 9,655 \text{ dm}^3 \cdot \text{mol}^{-1}$, and very good selectivity of binding for **1** as a result of change in solvent polarity, viz., $K_{\text{PC70BM-1 (Toluene)}}/K_{\text{PC70BM-1 (Mixed Solvent)}} \sim 3.0$. Due to solvophobic effect, the selectivity in binding for **2** in two different solvents, i.e., $K_{\text{PC70BM-2 (Toluene)}}/K_{\text{PC70BM-2 (Mixed Solvent)}}$ estimated to be ~ 1.0 . Lifetime measurements establish that static quenching mechanism is operative behind the photoexcited decay of **1**^{*} (and/ **2**^{*}) in presence of PC₇₀BM both in toluene and in mixed solvent. However, in mixed solvent, PC₇₀BM-**1** system is found to exhibit much higher value of magnitude of rate constant of charge-separation (i.e., $k_{\text{CS}}^{\text{s}}(\text{PC70BM-1}) = 2.97 \times 10^7 \text{ sec}^{-1}$ and $k_{\text{CS}}^{\text{s}}(\text{PC70BM-2}) = 5.60 \times 10^6 \text{ sec}^{-1}$) and quantum yield of charge-separation ($\phi_{\text{CS}}(\text{PC70BM-1}) = 0.070$) compared to PC₇₀BM-**2** system ($\phi_{\text{CS}}(\text{PC70BM-1}) = 0.015$). *Ab initio* calculations in *vacuo* predict the geometric structures of PC₇₀BM-**1** and PC₇₀BM-**2** systems and provide very good support in favour of charge-separation in former system in terms of multipole moment calculations.

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