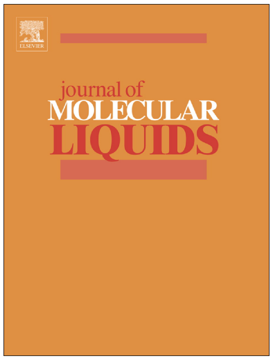

Molecular complexation between PCBM and porphyrazine in solution: A case study of non-covalent interaction

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

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Abstract

The present investigations report the non-covalent interaction of a fullerene derivative, namely, [6,6]-phenyl C_{71} butyric acid methyl ester ($PC_{70}BM$) 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 $PC_{70}BM$-**1** and $PC_{70}BM$-**2** systems in toluene, i.e., $K_{\text{PCBM-}\mathbf{1}} = 10{,}820\ \text{dm}^3\cdot\text{mol}^{-1}$ and $K_{\text{PCBM-}\mathbf{2}} = 9{,}655\ \text{dm}^3\cdot\text{mol}^{-1}$, and very good selectivity of binding for **1** as a result of change in solvent polarity, viz., $K_{\text{PC70BM-}\mathbf{1}\ \text{(Toluene)}}/K_{\text{PC70BM-}\mathbf{1}\ \text{(Mixed Solvent)}} \sim 3.0$. Due to solvophobic effect, the selectivity in binding for **2** in two different solvents, i.e., $K_{\text{PC70BM-}\mathbf{2}\ \text{(Toluene)}}/K_{\text{PC70BM-}\mathbf{2}\ \text{(Mixed Solvent)}}$ estimated to be ~1.0. Lifetime measurements establish that static quenching mechanism is operative behind the photoexcited decay of $\mathbf{1}^*$ (and/ $\mathbf{2}^*$) in presence of $PC_{70}BM$ both in toluene and in mixed solvent. However, in mixed solvent, $PC_{70}BM$-**1** system is found to exhibit much higher value of magnitude of rate constant of charge-separation (i.e., $k_{CS}{}^{s}{}_{(\text{PC70BM-}\mathbf{1})} = 2.97 \times 10^{7}\ \text{sec}^{-1}$ and $k_{CS}{}^{s}{}_{(\text{PC70BM-}\mathbf{2})} = 5.60 \times 10^{6}\ \text{sec}^{-1}$) and quantum yield of charge-separation ($\phi_{\text{CS(PC70BM-}\mathbf{1})} = 0.070$) compared to $PC_{70}BM$-**2** system ($\phi_{\text{CS(PC70BM-}\mathbf{1})} = 0.015$). *Ab initio* calculations in *vacuo* predict the geometric structures of $PC_{70}BM$-**1** and $PC_{70}BM$-**2** systems and provide very good support in favour of charge-separation in former system in terms of multipole moment calculations.