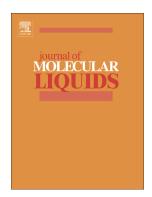
Accepted Manuscript

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



Anamika Ray, Sumanta Bhattacharya

PII: S0167-7322(17)33414-1

DOI: https://doi.org/10.1016/j.molliq.2017.12.093

Reference: MOLLIQ 8389

To appear in: Journal of Molecular Liquids

Received date: 28 July 2017

Revised date: 16 December 2017 Accepted date: 19 December 2017

Please cite this article as: Anamika Ray, Sumanta Bhattacharya, Molecular complexation between PCBM and porphyrazine in solution: A case study of non-covalent interaction. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), https://doi.org/10.1016/j.molliq.2017.12.093

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

ACCEPTED MANUSCRIPT

Molecular complexation between PCBM and porphyrazine in solution: a case study of noncovalent 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-5,10,15,20tetraaza-21H,23H-porphine (1) and zinc-2,7,12,17-tetra-tert-butyl-5,10,15,20-tetraaza-21H,23Hporphine (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_{PCBM-1} = $10.820 \text{ dm}^3 \cdot \text{mol}^{-1}$ and $K_{PCBM-2} = 9.655 \text{ dm}^3 \cdot \text{mol}^{-1}$, and very good selectivity of binding for 1 as a result of change in solvent polarity, viz., $K_{PC70BM-1 \text{ (Toluene)}}/K_{PC70BM-1 \text{ (Mixed Solvent)}} \sim 3.0$. Due to solvophobic effect, the selectivity in binding for 2 in two different solvents, i.e., K_{PC70BM-2} $(Toluene)/K_{PC70BM-2}$ (Mixed Solvent) estimated to be ~1.0. Lifetime measurements establish that static quenching mechanism is operative behind the photoexcited decay of $\boldsymbol{1}^*$ (and/ $\boldsymbol{2}^*$) 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., $k_{\text{CS}}^{\text{s}}_{\text{(PC70BM-1)}} = 2.97 \times 10^7 \text{ sec}^{-1} \text{ and } k_{\text{CS}}^{\text{s}}_{\text{(PC70BM-2)}} = 5.60 \times 10^6 \text{ sec}^{-1}) \text{ and quantum yield of}$ charge-separation ($\phi_{CS(PC70BM-1)} = 0.070$) compared to PC₇₀BM-2 system ($\phi_{CS(PC70BM-1)} = 0.015$). 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.

Download English Version:

https://daneshyari.com/en/article/7843056

Download Persian Version:

https://daneshyari.com/article/7843056

<u>Daneshyari.com</u>