



Molecular selectivity of indenopyridines for fullerenes: A comparative study

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ABSTRACT

Selectivity of [60]-Fullerene (C_{60}) over its [70]-analogue (C_{70}) is ably established for N-containing polynuclear aromatic planar indenopyridines (I) in organic media for the first time. The present work envisages the chemical physics behind non-covalent interaction between [70]-fullerene (C_{70}) and indenopyridines (I: I1, I3 and I4) in toluene alongwith a comparative analysis of previously studied interaction of C_{60} (Pal et al., 2019) via formation of multiple absorption isosbestic points and isoemissive point in UV-Vis and steady state fluorescence studies respectively, stable ground state equilibrium between C_{70} and I is recognized and is purely non-covalent in nature. All three indenopyridines showed high formation constant ($\sim 10^5$) with [70]-fullerene though the selectivity of binding favours [60]-fullerene. Experimental findings are well supported within *vacuo* DFT based computation. Loss of planarity of indenopyridines in the optimized adducts, FMO features, electrochemical indices and finally TD-DFT calculation validates the strong complexation. Taut wrapping of C_{70} by indenopyridines is most conspicuous for I4 among others as that of C_{60} .

1. Introduction

Huge studies has already been made in the field of charge transfer or electron donor-acceptor type weak interaction captivating Fullerenes viz. C_{60} and C_{70} as electron acceptor [1–12]. The exploration of the emission and optical properties of fullerenes and their derivatives is a central topic among the dynamic research fields of fullerenes to study charge separation recombination phenomena in energy storage devices [12]. These studies are gently related to “donor-acceptor” molecular systems in polynuclear aromatic compounds [13–23]. Varieties of donors are available in literature for which comparative efficiency of charge transfer interaction reported in organic media for Fullerenes [1–6].

N-containing polynuclear aromatic donor indenopyridine [18–21] plays noteworthy chemical and biological consequence. The efficiency of indenopyridines to form a weak binding complex with C_{60} has already been reported by our group [9]. To the best of our knowledge, there is no report of its comparative interaction with other fullerenes as electron acceptors till date. So the purpose of this study is to investigate the mode and efficiency of interaction of indenopyridine donors with [70]-fullerene acceptor in comparison with its [60]-analogue.

In this study better selectivity of C_{60} for indenopyridine donors are established through the formation of reaction equilibrium between [70]-

fullerene and three different indenopyridines viz., I1, I3 & I4 (Fig. 1). As that of C_{60} /I interactions reported earlier [9] all these are well established via the formation of both absorption isosbestic and isoemissive in toluene medium. Furthermore the interaction in the complex is modelled with density based change in global minimum geometry, Frontier orbital features, electrochemical indices and finally by TD-DFT transition estimation.

2. Experimental

2.1. Materials

Toluene HPLC (Merck India) grade is used as solvent. I1, I3 & I4, Indenopyridines are synthesized as reported [24], used in this study. Aldrich made [70]-fullerene (C_{70}) is used. The concentration range of 10^{-5} M – 10^{-6} M of indenopyridines (I1, I3 & I4) is taken and the range of 10^{-6} M are taken for C_{70} in all the spectral measurements.

2.2. Instruments used

The UV-Vis spectral measurements are performed using Shimadzu UV 2400 series PC spectrophotometer fitted with an electronic

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