

Azulene and naphthalene polymers

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There is strong interest in the application of polyazulenes and polynaphthalenes as materials have unique electrochemical and nonlinear optical properties that make applications possible in the fabrication of sensors, batteries, and electrochromic and electroluminescence devices [1,2]. Azulene is an aromatic compound isomer of naphthalene, although naphthalene and azulene are structurally similar with the same number of carbon and hydrogen atoms and 10 π -electrons, the properties of the azulene molecule differ from that of its isomer in many respects. The azulene molecule consists of fused five and seven membered rings, exhibits a large dipole moment $\mu=1.08D$ and an intense blue color, on the contrary, naphthalene molecule consists of two fused six membered rings with zero dipole moment and colorless appearance [3-5]. In the present work, we propose a theoretical study of a small polymer chain up to 10 azulene and naphthalene monomers in C_1 symmetry according to Fig.1.

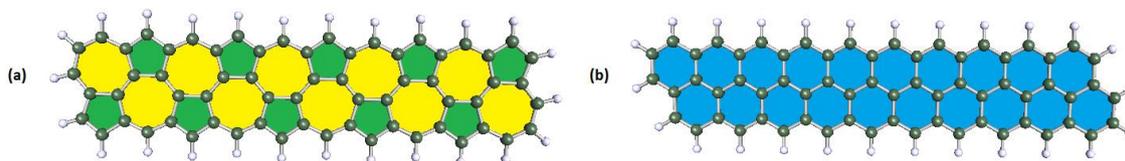


Fig.1 – Polymers: (a) [10]-azulene and (b) [10]-naphthalene

All calculations have been performed with TURBOMOLE software [6]. Calculations on the electronic ground state were carried out by Density Functional Theory (DFT), B3LYP/6-311G**. The [n]-naphthalene polymers are energetically more stable than the [n]-azulene ones. HOMO-LUMO energy gaps decrease as the polymer chain grows as shown in Fig.2.

The peaks of electronic transitions in the visible region (see Fig.3) are attributed to the small HOMO-LUMO energy gap, due to the extension of the π -electron system.



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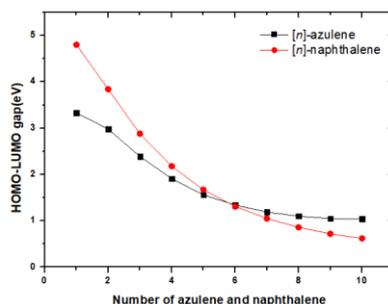


Fig.2 – HOMO-LUMO gap for [n]-azulene and [n]-naphthalene

We observed a shift of the maximum absorption peaks ($\pi \rightarrow \pi^*$ transition), from the visible region to the infrared, increasing polymer chains.

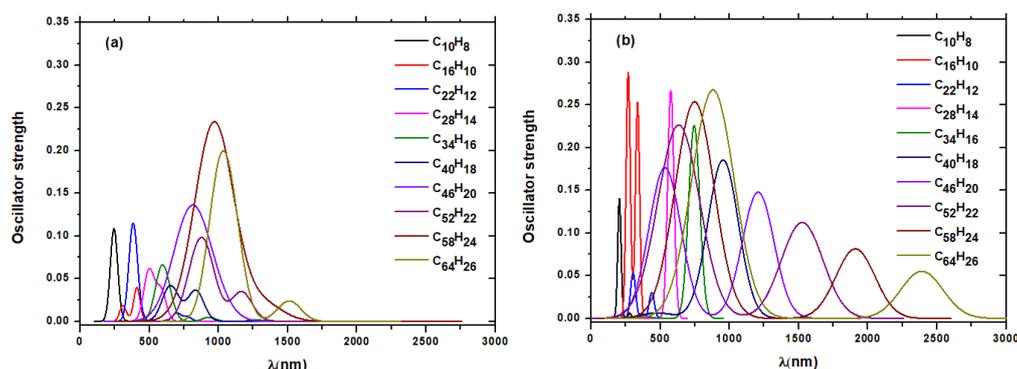


Fig.3 – UV-Vis spectra: (a) [n]-azulene and (b) [n]-naphthalene

Key-words: Density Functional Theory, Polyazulenes, Polynaphthalene

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