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TOPOLOGICAL DESCRIPTORS OF H-NAPHTALENIC NANOTUBES

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Topological descriptors are the numerical indices based on the topology of the atoms and their bonds (chemical conformation, quartenary structure). In this paper, counting topological descriptor called "szeged index", of H-naphtalenic nanotubes is strong-minded.

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1. Introduction

Since their discovery, by Iijima[1, 2] in 1991, carbon nanotubes have attracted increasing interest. The properties (mechanica[1, 3] optica [1, 4, 5] electronic [6-9] magnetic[10] or biological[11]) predicted or demonstrated for these tubular graphenes could have a beneficial impact in various areas of science and technology. Single-walled carbon nanotubes (SWNTs) have been isolated from the soot of vaporized graphite and visualized by electronic microscopy. Various physical and constitutional characteristics have been experimentally measured. Chemical functionalization [12-14] and doping [15, 16] results in significant changes of their initial properties.

Open SWNTs as well as capped tubes (according to isolated pentagon rule, IPR[17]) have been observed. "Circle crops" structures were first observed by Liu *et. at*.[18] and then by other groups.[19-21] Martel *et al*.20 argued that the observed rings were coils rather than perfect tori, but the structure composed from a toroidal tessellation of hexagonal rings has continued to attract a multitude of theoretical studies, dealing with construction, mathematical and physical properties of graphitic tori. [10]

Our previous papers focused on the topological descriptor of H-naphtalenic nanotubes.A topological descriptor are the numerical indices based on the topology of the atoms and their bonds (chemical conformation, quartenary structure).

First application of graph-theoretical invariants in studies of structure-properties relationship (QSPR) was proposed by Weiner [22]. However, it was after Randic [23] proposed atopological index for characterization of molecular branching, Randic index [24], that dramatic expansion of studies in the area started. There are more than one hundred topological indices which enables us to characterize the physicochemical properties of most of molecules.

The Szeged index is another topological index which is introduced by Ivan Gutman.[25-28] To define the Szeged index of a graph G, we assume that e = uv is an edge connecting the vertices u and v. Suppose N_u (e|G) is the number of vertices of G lying closer to u and N_v (e|G) is the number of vertices of G lying closer to v. Edges equidistance from u and v are not taken into account. Then the Szeged index of the graph G is defined as $Sz(G) = \sum_{e=uv\in E(G)} N_u(e|G)N_v(e|G)$, see also Ref [29].

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In Refs. [29-34] the PI and Szeged indices of some hexagonal graphs containing nanotubes and nanotorus are computed. In this paper, we continue this work to counting topological descriptor called "szeged index", of H-naphtalenic nanotubes and nanotori is strong-minded.

Our notation is standard and mainly taken from Refs [35,36].

2. Results and discussion

By close analogy to the phenylenic net, we propose now the naphthylenic net, with the sequence: C_6, C_6, C_4, C_6, and C_6... C_6, C_6, C_4, C_6, C_6, and the repeat unit C_6, C_6, C_4. The two naphthylenic patterns: HNP and HNPX were designed as shown in Figure 1. The corresponding *v*cutting nets are named VNP and VNPX. Following Diudea [37] we denote a H-naphtalenic nanotube by T=NPHX [2m, 2n]. In the following theorem we compute the Szeged index of the molecular graph *T* in Fig. 2.

Theorem 1. $Sz(T)= 2400n^3-10000n^3m-400n^2m^2+1200m^3n^2+8200m^4n^2+24\mu^2m+960\mu m^2n(n-m)^2+480\mu m^2|n-m|n+7200n^3m^2+6400n^3m^3-480\mu m^2n-8\mu^2 m|n-m|-48\mu^2 m(n-m)^2-64\mu^2 m(n-m)^3$; where

$$\mu = \begin{cases} 2mn & if\ m \geq n \\ 2mn-1 & if\ m< n \end{cases}$$

Proof. To compute the szeged index of T, we assume that A, B and C to be the set of all vertical, oblique and horizontal edges, respectively. Then we have:

$$\sum_{e\in C} N_u(e)N_v(e) + \sum_{e\in B} N_u(e)N_v(e) + \sum_{e\in A} N_u(e)N_v(e) = Sz(T) = \sum_{e\in E} N_u(e)N_v(e)$$

$$+\sum_{i=1}^{2m-1} 10n(i+2)(40mn-10n(i+2)(6n) += \sum_{i=1}^{2m} 10n(i+1)(40mn-10n(i+1)(6n)$$

$$\sum_{e\in C} N_u(e)N_v(e) + 2\sum_{i=1}^{2m-1} 5n(2i+m)(40mn-5n(2i+m)(6m)$$

So, to compute Sz(T), it is enough to obtaine last summation .Now suppose that e = uv be an oblique edge on i^{th} rows of molecular graph T. So that:

$N_u(e) = 2\mu(i+1)$; where $\mu = \begin{cases} 2mn & if\ m \geq n \\ 2mn-1 & if\ m< n \end{cases}$

and $\sum_{e\in C} N_u(e)N_v(e) = 2\sum_{i=1}^{2|m-n|-1} 2\mu(i+1)(40mn-2\mu(i+1)(3m)$

Thus $Sz(T)= 2400n^3-10000n^3m-400n^2m^2+1200m^3n^2+8200m^4n^2+24\mu^2m+960\mu m^2n(n-m)^2+480\mu m^2|n-m|n+7200n^3m^2+6400n^3m^3-480\mu m^2n-8\mu^2m|n-m|-48\mu^2 m(n-m)^2-64\mu^2m(n-m)^3$ ■

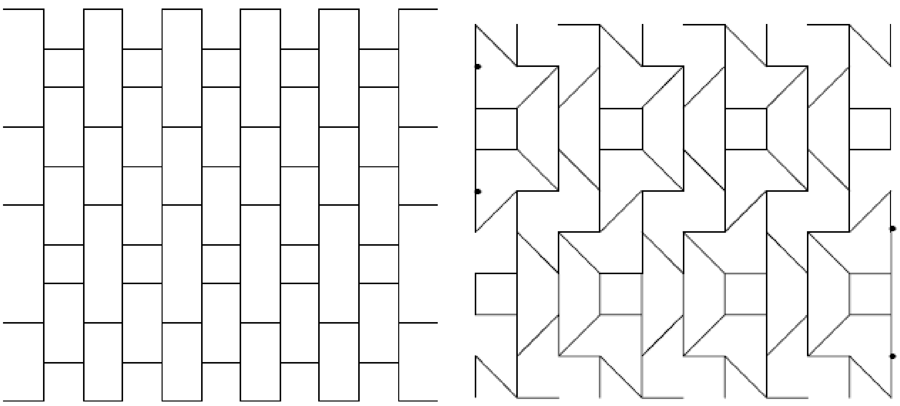

Fig. 1. Naphthylenic patterns derived from a square net.

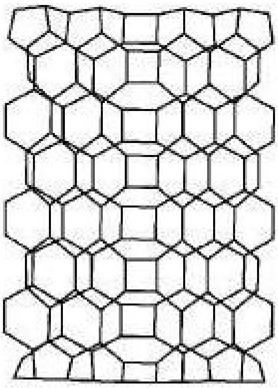

Fig. 2. Naphthylenic nanotubes (detail).

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