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Some degree based connectivity indices of nano-structures

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A topological index of a molecular graph *G* is a numeric quantity related to *G* which is invariant under symmetry properties of *G*. In the present study, several topological indices are computed in linear [*n*]-anthracene, *V* -anthracene nanotube and nanotori: Zagreb, Randić, Sum-connectivity, *GA*, *ABC* indices and Zagreb polynomials.

Keywords: Degree based topological indices, Molecular graphs, Linear [*n*]-anthracene, *V* –anthracene nanotube, *V* -anthracene nanotori.

INTRODUCTION

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph are called vertices and edges of the graph, respectively. A simple graph is an unweighed, undirected graph without loops or multiple edges. All graphs in this paper are simple. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted. In the past years, nano-structures involving carbon have been the focus of an intense research activity which is driven to a large extent by the quest for new materials with specific applications. A topological index is a real number that is derived from molecular graphs of chemical compounds. In organic chemistry, topological indices have been found to be useful in chemical documentation, isomer discrimination, structure-property relationships, structure-activity relationships (SAR) and pharmaceutical drug design. There has been considerable interest in the general problem of determining topological indices [1, 2, 3]. The main goal of this paper is to compute some topological indices and polynomials for a family of linear [*n*]-anthracene, lattice of *V*-anthracene nanotube and nanotori. The paper is organized as follows: firstly we give the necessary definitions and secondly we compute some topological indice values for the above mentioned nanotubes and nanotori.

DEFINITIONS

We now recall some algebraic definitions related to the topological indices chosen for the present study. A graph *G* consists of a set of vertices *V* (*G*) and a set of edges *E* (*G*). The vertices in *G* are connected by an edge if there exists an edge $uv \in E\ (G)$ connecting the vertices *u* and *v* in *G* such that $u, v\ \in V\ (G)$. The degree d_u of a vertex $u \in V\ (G)$ is the number of vertices of *G* adjacent to *u*. There are several topological indices already defined.

The *first Zagreb index* and the *second Zagreb index* have been introduced more than thirty years ago by Gutman and Trinajstić [4]. They respectively are defined as:

$$M_1\ (G) = \sum_{u \in V\ (G)} (d_u)^2\ , M_2\ (G) = \sum_{uv \in E(G)} d_u d_v$$

In fact, one can rewrite the *first Zagreb index* as:

$$M_1\ (G) = \sum_{uv \in E(G)} (d_u + d_v)$$

The product-connectivity index, also called *Randić index* of a graph *G* and is defined such as:

$$\chi\ (G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

This topological index was first proposed by Randić [5] in 1975. In 2009, Zhou and Trinajstić [6] proposed another connectivity index, named the *Sum-connectivity index*. This index is defined as follows:

$$X\ (G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}$$

The *geometric-arithmetic* (*GA*) *index* is another topological index based on degrees of vertices defined by Vukičević and Furtula [7]:

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

Estrada et al. [8] introduced the *atom-bond connectivity* (*ABC*) *index*, which has been applied

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to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u\, d_v}}$$

Recently, Fath-Tabar [9] put forward the *first and the second Zagreb polynomials* of the graph *G*, defined respectively as:

$$ZG_1\,(G, x) = \sum_{uv \in E(G)} x^{d_u + d_v},$$

$$ZG_2\,(G, x) = \sum_{uv \in E(G)} x^{d_u d_v}$$

where *x* is a dummy variable.

RESULTS AND DISCUSSION

In this section, at first, we compute index for anthracene graph. Anthracene is a solid polycyclic aromatic hydrocarbon of formula C_{14} H_{10}, consisting of three fused benzene rings. It is a component of coal tar. Anthracene is used in the production of the red dye alizarin and other dyes.

Example 3.1. Let *G* be the anthracene graph (Figure 1), there are three types of edges, e. g. edges with endpoints 2 [E_1], edges with endpoints 2, 3 [E_2] and edges with endpoints 3 [E_3].

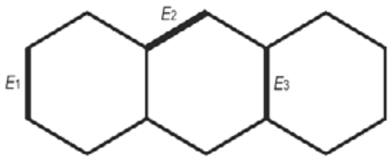

Fig.1. Basic structure of an anthracene

These edges are enumerated as 6, 8 and 2 edges of types 1, 2 and 3, respectively.

(i) $M_1\,(G) = \sum_{uv \in E(G)} (d_u + d_v) = \sum_{uv \in E_1} (2+2) + \sum_{uv \in E_2} (2+3) + \sum_{uv \in E_3} (3+3) = 4 \times 6 + 5 \times 8 + 6 \times 2 = 76$

(ii) $M_2\,(G) = \sum_{uv \in E(G)} (d_u \times d_v) = \sum_{uv \in E_1} (2 \times 2) + \sum_{uv \in E_2} (2 \times 3) + \sum_{uv \in E_3} (3 \times 3) = 4 \times 6 + 6 \times 8 + 9 \times 2 = 90$

(iii) $\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}} = \sum_{uv \in E_1} \frac{1}{\sqrt{2 \times 2}} + \sum_{uv \in E_2} \frac{1}{\sqrt{2 \times 3}} + \sum_{uv \in E_3} \frac{1}{\sqrt{3 \times 3}} = \frac{1}{2} \times 6 + \frac{1}{\sqrt{6}} \times 8 + \frac{1}{3} \times 2 = \frac{11 + 4\sqrt{6}}{3}.$

(iv) $X(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} = \sum_{uv \in E_1} \frac{1}{\sqrt{2+2}} + \sum_{uv \in E_2} \frac{1}{\sqrt{2+3}} + \sum_{uv \in E_3} \frac{1}{\sqrt{3+3}} = \frac{1}{2} \times 6 + \frac{1}{\sqrt{5}} \times 8 + \frac{1}{\sqrt{6}} \times 2 = 3 + \frac{8\sqrt{5}}{5} + \frac{2\sqrt{6}}{6}.$

(v) $GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \sum_{uv \in E\,E_1} \frac{2\sqrt{2 \times 2}}{2+2} + \sum_{uv \in E_2} \frac{2\sqrt{2 \times 3}}{2+3} + \sum_{uv \in E_3} \frac{2\sqrt{3 \times 3}}{3+3} + = 6 + \frac{2\sqrt{6}}{5} \times 8 + 2 = 3 + \frac{40 + 16\sqrt{6}}{5}.$

(vi) $ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} + \sum_{uv \in E_1} \sqrt{\frac{2+2-2}{2 \times 2}} + \sum_{v \in E_1} \sqrt{\frac{2+3-2}{2 \times 3}} + \sum_{uv \in E_3} \sqrt{\frac{3+3-2}{3 \times 3}} = \sqrt{\frac{2}{4}} \times 6 + \sqrt{\frac{3}{6}} \times 8 + \sqrt{\frac{4}{9}} \times 2 = 7\sqrt{2} + \frac{4}{3}.$

Now we compute first Zagreb, second Zagreb, product-connectivity, sum-connectivity, geometric-arithmetic and atom-bond connectivity indices of a linear [*n*]-anthracene, as described in Example 3.1.

It is seen that *T* = *T*[*n*] has 14*n* vertices and 18*n*-2 edges and the edge set of the graph can be divided in three partitions, e. g. $E_1(T)$, $E_2(T)$ and $E_3(T)$. The following table gives the three types and gives the number of edges in each type.

From table 1, we give an explicit formula for some indices of a linear [*n*]-anthracene, as shown in Figure 2.

Table 1. Computing the Number of edges for a linear [*n*]-Anthracene**.**

(d_u , d_v) where $uv \in E\ (T)$	Total Number of edges
$E_1 = [2, 2]$	6
$E_2 = [2, 3]$	12n-4
$E_3 = [3, 3]$	6n-4

Theorem 3.2. Consider the graph *T of* a linear [*n*]-*Anthracene.* Then

(i) $M_1\,(T) = \sum_{uv \in E\,(G)} (d_u + d_v) = \sum_{uv \in E_1} 4 + \sum_{uv \in E_2} 5 + \sum_{uv \in E_3} 6 = 4 \times 6 + 5 \times (12n - 4) + 6 \times (6n - 4) = 96n - 20.$

(ii) $M_2\,(T) = \sum_{uv \in E\,(T)} (d_u d_v) = \sum_{uv \in E_1} 4 + \sum_{uv \in E_2} 6 + \sum_{uv \in E_3} 9 = 4 \times 6 + 6 \times (12n - 4) + 9 \times (6n - 4) = 126n - 36.$

(iii) $\chi(T) = \sum_{uv \in E\,(T)} \frac{1}{\sqrt{d_u d_v}} = \sum_{uv \in E_1} \frac{1}{\sqrt{4}} + \sum_{uv \in E_2} \frac{1}{\sqrt{6}} + \sum_{uv \in E_3} \frac{1}{\sqrt{9}} = \frac{1}{\sqrt{4}} \times 6 + \frac{1}{\sqrt{6}} \times (12n - 4) + \frac{1}{\sqrt{9}} \times (6n - 4) = \left(2 + 2\sqrt{6}\right)n + \left(\frac{5 + 2\sqrt{6}}{3}\right).$

(iv) $X(T) = \sum_{uv \in E\,(t)} \frac{1}{\sqrt{d_u + d_v}} = \sum_{uv \in E_1} \frac{1}{\sqrt{4}} + \sum_{uv \in E_2} \frac{1}{\sqrt{5}} + \sum_{uv \in E_3} \frac{1}{\sqrt{6}} = \frac{1}{\sqrt{4}} \times 6 + \frac{1}{\sqrt{5}} \times (12n - 4) + \frac{1}{\sqrt{6}} \times (6n - 4) = \left(12\sqrt{5} + \sqrt{6}\right)n + (3 - \frac{2\sqrt{6}}{3} - \frac{4\sqrt{5}}{5}).$

(v) $GA(T) = \sum_{uv \in E\,(T)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} = \sum_{uv \in E_1} \frac{2\sqrt{4}}{4} + \sum_{uv \in E_2} \frac{2\sqrt{6}}{5} + \sum_{uv \in E_3} \frac{2\sqrt{9}}{6} + = \frac{2\sqrt{4}}{4} \times 6 + \frac{2\sqrt{6}}{5} \times (12n - 4) + \frac{2\sqrt{9}}{6} \times (6n - 4) = \left(6 + \frac{24\sqrt{6}}{5}\right)n + \left(2 - \frac{8\sqrt{6}}{5}\right).$

Fig. 2. The molecular graph of a linear [n]-anthracene.

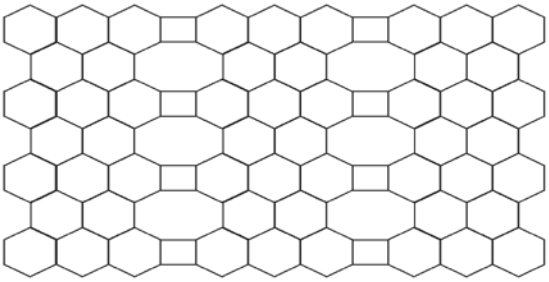

Fig.3. The 2-D graph lattice of $G=G[p,q]$ with $p= 3$ and $q= 4$.

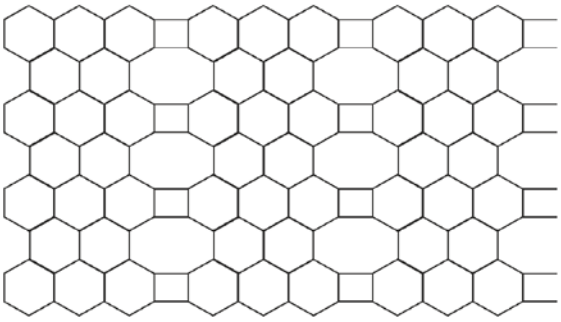

Fig. 4. The 2-D graph lattice of $K=K[p,q]$ with $p= 3$ and $q= 4$

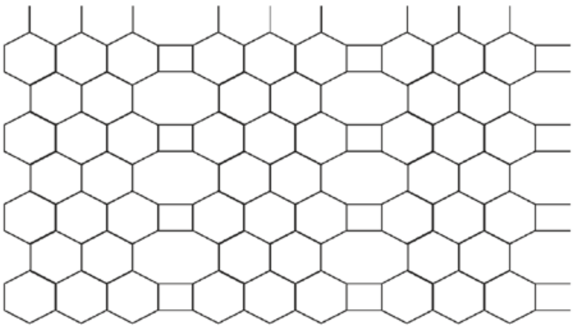

Fig. 5. The 2-D graph lattice of $L=L[p,q]$ with $p= 3$ and $q= 4$.

Theorem 3.3. Let G be a 2-dimensional lattice of V-anthracene (see Figure 3), K *be a* lattice of V-anthracene nanotube (see Figure 4) and L *be a* lattice of V-anthracene nanotori (see Figure 5). Then,
$|V(G)| = |V(K)| = |V(L)| = 14pq$, $|E(G)| = 21pq - 3p - 2q$, $|E(K)| = 21pq - 3p$ and $|E(L)| = 21pq$.

From table 2, we give an explicit computing formula for some indices of lattice of V–anthracene nanotube and nanotori, as shown in Figures 3, 4 and 5.

In graph theory, a regular graph is a graph where each vertex has the same number of neighbors, i.e. every vertex has the same degree or valency. A regular graph with vertices of degree k is called a k-regular graph or regular graph of degree k. Now, we need the following lemma to calculate the indices of L:

Lemma 3.4. Let G be an *arbitrary graph.* Then G is *k-regular* if and only if one of the followings hold:

1. $M_1(G) = 2\kappa\,|E(G)|$.
2. $M_2(G) = \kappa^2|E(G)|$.
3. $\chi(G) = \frac{1}{\kappa}|E(G)|$.
4. $X(G) = \frac{1}{\sqrt{2\kappa}}|E(G)|$.
5. $GA(G) = |E(G)|$.
6. $ABC(G) = \frac{\sqrt{2(\kappa-1)}}{\kappa}|E(G)|$

Table 2. Computing the number of edges for molecular graph G, K and L.

(d_u, d_v) where $uv \in E$	Number of Edges G	Number of Edges K	Number of Edges L
$E_1 = [2,2]$	2q+4	0	0
$E_2 = [2,3]$	12p+4q-8	12p	0
$E_3 = [3,3]$	21pq-15p-8q+4	21pq-15p	21pq

Table 3. Topological indices for the molecular graphs of Figures 3 and 4.

Index	Graph G	Graph K
M_1	$126pq-30p-20q$	$126pq-30p$
M_2	$189pq-63p-40q+4$	$189pq-63p$
χ	$7pq+(2\sqrt{6}-5)p+(\frac{2\sqrt{6}-5}{3})q+(\frac{10-4\sqrt{6}}{3})$	$7pq+(2\sqrt{6}-5)p$
X	$\frac{7\sqrt{6}}{2}pq+(\frac{12\sqrt{5}}{5}-\frac{5\sqrt{6}}{2})p+(1+\frac{4\sqrt{5}}{5}-\frac{4\sqrt{6}}{3})q+(2-\frac{8\sqrt{5}}{5}+\frac{2\sqrt{6}}{3})$	$\frac{7\sqrt{6}}{2}pq+(\frac{12\sqrt{5}}{5}-\frac{5\sqrt{6}}{2})p$
GA	$21pq+(\frac{24\sqrt{6}}{5}-15)p+(\frac{8\sqrt{6}}{5}-6)q+(8-\frac{16\sqrt{6}}{5})$	$21pq+(\frac{24\sqrt{6}}{5}-15)p$
ABC	$14pq+(6\sqrt{2}-10)p+(3\sqrt{2}-\frac{16}{3})q+(\frac{8}{3}-2\sqrt{2})$	$14pq+(6\sqrt{2}-10)p$

Proof. It is easy to check according to Figure 5. By using Lemma 3.4, consider the Figure 5. We can see that V -anthracene nanotori graph is 3-regular. So, we illustrate these results in the table below:

Table 4. Topological indices for the molecular graphs of Fig. 5.

Index	Graph L
M_1	**126 pq**
M_2	**189pq**
χ	**7pq**
X	$\frac{7\sqrt{6}}{2}$ **pq**
GA	**21pq**
ABC	**14pq**

Finally, we will calculate the first and second Zagreb polynomials of the above molecular graphs.

Theorem 3.5. The first and second Zagreb polynomials of the above graphs are computed as follows:

(i) $ZG_1(G, x) = (12pq - 15p - 8q + 4)\,x^6 + (12p + 4q - 8)\,x^5 + (2q + 4)\,x^4$,

(ii) $ZG_2(G, x) = (21pq - 15p - 8q + 4)\,x^9 + (12p + 4q - 8)\,x^6 + (2q + 4)\,x^4$,

(iii) $ZG_1(K, x) = (21pq - 15p)\,x^6 + (12p)\,x^5$,

(iv) $ZG_2(K, x) = (21pq - 15p)\,x^9 + (12p)\,x^6$,

(v) $ZG_1(L, x) = (21pq)\,x^6$,

(vi) $ZG_2(L, x) = (21pq)\,x^9$.

Proof. By definition of Zagreb polynomials, the proof is clear.

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НЯКОИ СТЕПЕННО БАЗИРАНИ ИНДЕКСИ НА СВЪРЗВАНЕ НА НАНОСТРУКТУРИ

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(Резюме)

Топологичният индекс на молекулен граф G е число, свързано с G, който е инвариантно по симетрични свойства на G. В настоящото проучване се изчисляват няколко топологични индекси за линеен [n] антрацен, V-антрацен, нанотръба и нанотори: Загреб, Рандич, сума на свързаност, GA, ABC индекси и Загреб полиноми.