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THEORETICAL STUDY OF NANOSTRUCTURES USING TOPOLOGICAL INDICES

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ABSTRACT. In this research, we give some theoretical results for linear $[n]$-Pentacene, V-Pentacenic nanotube, H-Pentacenic nanotube and V-Pentacenic nanotori by using topological indices. The main result of this paper is represented by the formulas for calculating values of Zagreb indices, Zagreb coindices and connectivity indices. These formulas make it possible to correlate the chemical structure of Nanostructures with a large amount of information about their physical features.

Keywords: *Nanostructures, Vertex-degree, Zagreb indices, Zagreb coindices, Connectivity indices.*

INTRODUCTION

The chemical graph theory is an important branch of mathematical chemistry. A chemical graph is a model of a chemical system, used to characterize the interactions among its components: atoms, bonds, groups of atoms or molecules. A structural formula of a chemical compound can be represented by a molecular graph, its vertices being atoms while edges correspond to covalent bonds; hydrogen atoms are often omitted. A single number, representing a chemical structure, in graph-theoretical terms, is called a topological index. Topological indices were successfully employed in developing a suitable correlation between chemical structure and biological activity by translating chemical structures into numerical descriptors. In the past years, nanostructures 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. Carbon nanotubes are nano-objects that have raised great expectations in a number of different applications, including field emission, energy storage, molecular electronics, atomic force microscopy, and many others. The use of topological indices as structural

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descriptors is important in the proper and optimal nanostructure design. The present authors, [1-6], derived some exact formulae for topological indices of some graphs.

The main purpose of this paper is to compute some topological indices for families of linear [n]-Pentacene, lattice of V-Pentacenic nanotube, H-Pentacenic nanotube and V-Pentacenic nanotori. The paper is organized as follows: In the next sections we give the necessary definitions. Section 3 contains the results; the paper is completed with the list of references.

DEFINITIONS

In this section, we gathered some notations as well as preliminary notions which will be needed for the rest of the paper. Let $G = (V, E)$ be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge sets of it being represented by $V = V(G)$ and $E = E(G)$, respectively. 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 complement of G, denoted by $\overline{\mathrm{G}}$, is a simple graph on the same set of vertices $V(G)$ in which two vertices u and v are adjacent, i.e., connected by an edge uv, if and only if they are not adjacent in G. Hence, $uv \in E(\bar{G}) \Leftrightarrow uv \notin E(G)$. The degree of $u \in V(G)$, denoted by d_u, is the number of vertices in G adjacent to u. There are several topological indices defined in the literature.

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstić [7]. For a (molecular) graph G, the *first Zagreb index* is equal to the sum of the squares of the vertex degrees; the *second Zagreb index* equals to the sum of the products of pair adjacent vertex degrees. They are defined as:

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

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

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

The *first and second Zagreb polynomials* of a graph G are defined as:

$$M_1(G, x) = \sum_{uv \in E(G)} x^{(d_u + d_v)}, \qquad M_2(G, x) = \sum_{uv \in E(G)} x^{(d_u \times d_v)},$$

where x is a dummy variable. For more studies about polynomials in graph theory you can see [8-12].

On the other hand, for a graph G, the *modified second Zagreb index* is defined as [13]:

$$M_2^*(G) = \sum_{uv \in E(G)} \frac{1}{d_u \times d_v}$$

The *third Zagreb index* was first introduced by Fath-Tabar [14]. This index is defined as follows:

$$M_3(G) = \sum_{uv \in E(G)} |d_u - d_v|.$$

Recently, Ashrafi et al. [15] have defined, respectively, the *first Zagreb coindex* and the *second Zagreb coindex* as follows:

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} (d_u + d_v), \quad \overline{M_2}(G) = \sum_{uv \notin E(G)} (d_u \times d_v).$$

Zagreb coindices are dependent on the degrees of non-adjacent vertices and thereby quantifying a possible influence of remote vertex pairs to the molecular properties. The reader should note that Zagreb coindices of G are not Zagreb indices of $\bar{G}$; the defining sums run over $E(\bar{G})$, but the degrees are with respect to G.

Among molecular descriptors, topological connectivity indices are very important and many of them have found applications in modeling chemical, pharmaceutical and other properties of the molecules. The *product-connectivity index*, also called Randić index of a graph G and is defined as:

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

This topological index was first proposed by Randić [16]. Zhou and Trinajstić [17] proposed another connectivity index, named the *Sum-connectivity index*. This index is defined as:

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

Estrada et al. [18] introduced *atom-bond connectivity index*, which it has been applied in studies on the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows:

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

Vukičević and Furtula [19] proposed a topological index named the *geometric-arithmetic index*. This index is defined as:

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

RESULTS AND DISCUSSION

The use of topological and connectivity indices as structural descriptors is important in proper and optimal nanostructure design. Pentacene is a polycyclic aromatic hydrocarbon consisting of five linearly-fused benzene rings. This highly conjugated compound is an organic semiconductor. The compound generates excitons upon absorption of ultra-violet (UV) or visible light; this makes it very sensitive to oxidation. For this reason, this compound, which is a purple powder, slowly degrades upon exposure to air and light. In Figure1, one can see the linear [n]-Pentacene.

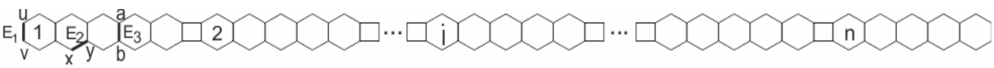

Figure 1. The molecular graph of a linear [n]-Pentacene.

Before we proceed to our main results, we will express the lemma which will be useful later.

Lemma 1.*Topological indices of [n]-Pentacene (Figure* 1*), hereafter* denoted *T=T*[*n*], *are calculated from the molecular graph, considering the vertex degree and the number of edges. Obviously, for* $n = 1, |V| = 22$ *and* $|E| = 26$. *There exist* 3 *type of edges, namely* $[E_1] = uv$, $[E_2] = xy$ *and* $[E_3] = ab$. *On the other hand* $d_u = d_v = 2$, $d_a = d_b = 3$ *and* $d_x = 2$, $d_y = 3$. *By enumerating these edges there are* $6, 16$ *and* 4 *edges of types* $1, 2$ *and* 3, *respectively. Now, it is easy to see that* $T = T[n]$ *has* $22n$ *vertices and* $28n - 2$ *edges. Similar to the above argument, the edge set of graph can be dividing into three partitions:* $E_1(T), E_2(T)$ *and* $E_3(T)$.*There are three type of edges, e. g. edges with endpoints* $2[E_1]$, *edges with endpoints* $2{,}3[E_2]$ *and edges with endpoints* $3[E_3]$. *By using an algebraic method we obtain* $|E_1| = 6$, $|E_2| = 20n - 4$ *and* $|E_3| = 8n - 4$.

Table 1. Type and number of edges in the molecular graph T

(d_u, d_v) where $uv \in E(T)$	Total Number of Edges
$E_1 = [2,2]$	6
$E_2 = [2,3]$	$20n - 4$
$E_3 = [3,3]$	$8n - 4$

Theorem 2. *Let T be a linear [n]-Pentacene; the Zagreb polynomials are:*

i. $M_1(T,x) = (8n-4)x^6 + (20n-4)x^5 + 6x^4$.
ii. $M_2(T,x) = (8n-4)x^9 + (20n-4)x^6 + 6x^4$.

Proof. By definition of the first and second Zagreb polynomials and partition of edges described in Lemma 1, we can see that:

i. $M_1(T,x) = \sum_{uv\in E(T)} x^{(d_u+d_v)} = \sum_{uv\in[E_1]} x^{4} + \sum_{uv\in[E_2]} x^{5} + \sum_{uv\in[E_3]} x^{6} = 6x^4 + (20n-4)x^5 + (8n-4)x^6$.
ii. $M_2(T,x) = \sum_{uv\in E(T)} x^{(d_u\times d_v)} = \sum_{uv\in[E_1]} x^{4} + \sum_{uv\in[E_2]} x^{6} + \sum_{uv\in[E_3]} x^{9} = 6x^4 + (20n-4)x^6 + (8n-4)x^9$.

Theorem 3. Let T *be a linear [n]-Pentacene; the topological indices are calculated from the corresponding polynomials as the first derivative, in* $x = 1$*:*

$$M_1(T) = 148n - 20.$$

$$M_2(T) = 192n - 36.$$

Proof.

The first Zagreb index will be the first derivative of $M_1(T,x)$ evaluated at $x = 1$:

$$M_1(T) = \left.\frac{\partial M_1(T,x)}{\partial x}\right|_{x=1} = 6\times(8n-4) + 5\times(20n-4) + 4\times(6) = 148n - 20.$$

Also, the second Zagreb index will be the first derivative of $M_2(T,x)$ evaluated at $x = 1$:

$$M_2(T) = \left.\frac{\partial M_2(T,x)}{\partial x}\right|_{x=1} = 9\times(8n-4) + 6\times(20n-4) + 4\times(6) = 192n - 36.$$

Given the edge partitions in the linear [n]-Pentacene (Lemma 1) we can prove the following theorem:

Theorem 4. *Consider the graph T of a linear [n]-Pentacene. The following topological indices can be calculated:*

i. $M_2^*(T) = \sum_{uv\in E(T)} \frac{1}{d_u \times d_v} = \sum_{uv\in[E_1]} \frac{1}{4} + \sum_{uv\in[E_2]} \frac{1}{6} + \sum_{uv\in[E_3]} \frac{1}{9} = \frac{1}{4} \times 6 + \frac{1}{6} \times (20n - 4) + \frac{1}{9} \times (8n - 4) = \frac{38}{9} n + \frac{7}{18}$.

ii. $M_3(T) = \sum_{uv\in E(T)} |d_u - d_v| = \sum_{uv\in[E_2]} |2-3| = 20n - 4$.

iii. $\chi(T) = \sum_{uv\in E(T)} \frac{1}{\sqrt{d_u d_v}} = \sum_{uv\in[E_1]} \frac{1}{\sqrt{4}} + \sum_{uv\in[E_2]} \frac{1}{\sqrt{6}} + \sum_{uv\in[E_3]} \frac{1}{\sqrt{9}} = \frac{1}{\sqrt{4}} \times 6 + \frac{1}{\sqrt{6}} \times (20n - 4) + \frac{1}{\sqrt{9}} \times (8n - 4) = \left(\frac{10\sqrt{6}+8}{3}\right) n + \left(\frac{5-2\sqrt{6}}{3}\right)$.

iv. $X(T) = \sum_{uv\in E(T)} \frac{1}{\sqrt{d_u + d_v}} = \sum_{uv\in[E_1]} \frac{1}{\sqrt{4}} + \sum_{uv\in[E_2]} \frac{1}{\sqrt{5}} + \sum_{uv\in[E_3]} \frac{1}{\sqrt{6}} = \frac{1}{\sqrt{4}} \times 6 + \frac{1}{\sqrt{5}} \times (20n - 4) + \frac{1}{\sqrt{6}} \times (8n - 4) = \left(4\sqrt{5} + \frac{4\sqrt{6}}{3}\right) n + \left(3 - \frac{4\sqrt{5}}{5} - \frac{2\sqrt{6}}{3}\right)$.

v. $ABC(T) = \sum_{uv\in E(T)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} = \sum_{uv\in[E_1]} \sqrt{\frac{2}{4}} + \sum_{uv\in[E_2]} \sqrt{\frac{3}{6}} + \sum_{uv\in[E_3]} \sqrt{\frac{4}{9}} = \sqrt{\frac{2}{4}} \times 6 + \sqrt{\frac{3}{6}} \times (20n - 4) + \sqrt{\frac{4}{9}} \times (8n - 4) = \left(\frac{16+30\sqrt{2}}{3}\right) n + \left(\frac{3\sqrt{2}-8}{3}\right)$.

vi. $GA(T) = \sum_{uv\in E(T)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} = \sum_{uv\in[E_1]} \frac{2\sqrt{4}}{4} + \sum_{uv\in[E_2]} \frac{2\sqrt{6}}{5} + \sum_{uv\in[E_3]} \frac{2\sqrt{9}}{6} = \frac{2\sqrt{4}}{4} \times 6 + \frac{2\sqrt{6}}{5} \times (20n - 4) + \frac{2\sqrt{9}}{6} \times (8n - 4) = \left(8 + 8\sqrt{6}\right) n + \left(2 - \frac{8\sqrt{6}}{5}\right)$.

Lemma 5. [15] Let G be a simple graph with n vertices. Then

i. $\overline{M_1}(G) = 2|E(G)|(n-1) - M_1(G)$.

ii. $\overline{M_2}(G) = 2|E(G)|^2 - M_2(G) - \frac{1}{2} M_1(G)$.

Theorem 6. *The first and second Zagreb coindices of a linear* [n]*-Pentacene are computed as:*

i. $\overline{M_1}(T) = 1232n^2 - 292n + 24$.

ii. $\overline{M_2}(T) = 1568n^2 - 490n + 54$.

Proof. By applying Lemma 1 and Lemma 5 we have the proof.

The 2-dimensional lattices of V-Pentacenic nanotube (denoted by $F = F[p,q]$), H-Pentacenic nanotube (denoted by $K = K[p,q]$) and V-Pentacenic nanotori (denoted by $L = L[p,q]$) the readers can see in Figures 2, 3 and 4, respectability.

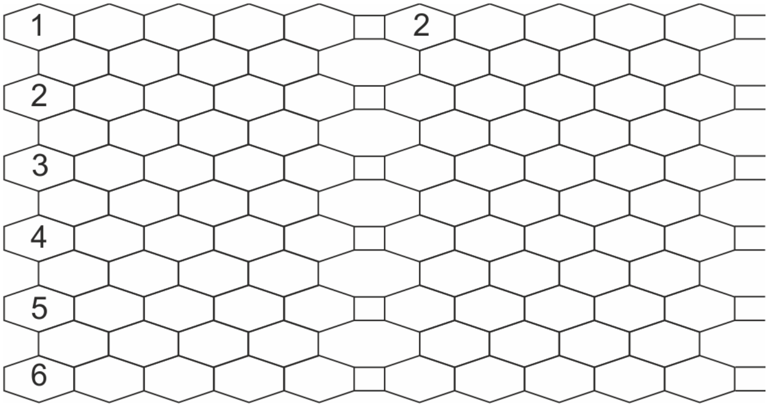

Figure 2. The 2-D graph lattice of $F = F[p, q]$ with $p = 2$ and $q = 6$.

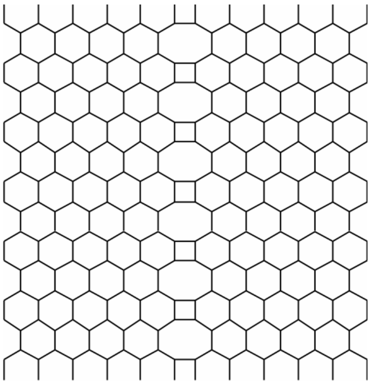

Figure 3. The 2-D graph lattice of $K = K[p, q]$ with $p = 2$ and $q = 6$.

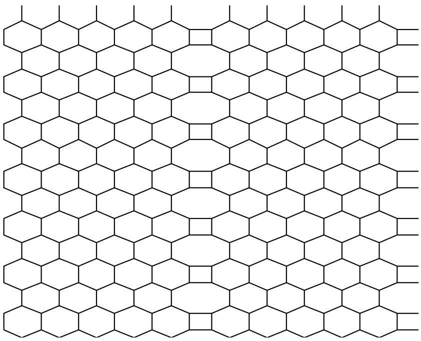

Figure 4. The 2-D graph lattice of $L = L[p, q]$ with $p = 2$ and $q = 7$.

In order to provide a unified approach to the results discussed in this paper, we express the following lemma.

Lemma 7. It holds that:

Table 2. Type and number of vertices and edges in the molecular graphs ***F***, ***K*** and ***L***.

Nanostructure	$\lvert V\rvert$	$\lvert E\rvert$	$\lvert E_1\rvert$	$\lvert E_2\rvert$	$\lvert E_3\rvert$
F	$22pq$	$33pq-5p$	0	$20p$	$33pq-25p$
K	$22pq$	$33pq-2q$	$2q$	$4q$	$33pq-8q$
L	$22pq$	$33pq$	0	0	$33pq$

Proof. We apply similar reasoning as in Lemma 1 to calculate the quantities of $|V|, |E_1|, |E_2|$ and $|E_3|$ of Nanostructures F, K and L.

Theorem 8. *The first, second, modified second and third Zagreb indices of Nanostructures are computed as:*

Nanostructure	M_1	M_2	M_2^*	M_3
F	$198pq-50p$	$297pq-105p$	$\frac{11}{3}pq+\frac{5}{9}p$	$20p$
K	$198pq-20q$	$297pq-40q$	$\frac{11}{3}pq+\frac{5}{18}p$	$4q$
L	$198pq$	$297pq$	$\frac{11}{3}pq$	0

Proof. We just apply Lemma 7 and the proof of Theorem 4.

Theorem 9. *The first and second Zagreb coindices of Nanostructures are calculated as:*

Nanostruc-ture	$\overline{M_1}$	$\overline{M_2}$
F	$1452p^2q^2-220p^2q-264pq+60p$	$2178p^2q^2-660p^2q+50p^2-396pq+130p$
K	$1452p^2q^2-88pq^2-264pq+24q$	$2178p^2q^2-264pq^2-396pq+58q$
L	$1452p^2q^2-264pq$	$2178p^2q^2-396pq$

Proof. The proof is obtained exactly from Lemma 5, Lemma 7 and Theorem 8.

Finally, we calculate the Randić index, Sum-connectivity index, atom-bond connectivity index and geometric-arithmetic index of Nanostructures by use an algebraic method. The next results are proven like Theorem 4 therefore, we omit the proofs.

Theorem 10. *The Product and Sum-connectivity indices are computed as:*

Nanostructure	χ	X
F	$11pq+\left(\frac{10\sqrt{6}-25}{3}\right)p$	$\frac{11\sqrt{6}}{2}pq+\left(\frac{120\sqrt{5}-125\sqrt{6}}{30}\right)p$
K	$11pq+\left(\frac{2\sqrt{6}-5}{3}\right)q$	$\frac{11\sqrt{6}}{2}pq+\left(\frac{30+24\sqrt{5}-40\sqrt{6}}{30}\right)q$
L	$11pq$	$\frac{11\sqrt{6}}{2}pq$

Theorem 11. *The* atom-bond connectivity index and geometric-arithmetic index *are computed as:*

Nanostructure	ABC	GA
F	$22pq+\left(10\sqrt{2}-\frac{50}{3}\right)p$	$33pq+\left(8\sqrt{6}-25\right)p$
K	$22pq+\left(3\sqrt{2}-\frac{16}{3}\right)q$	$33pq+\left(\frac{8\sqrt{6}}{5}-6\right)q$
L	$22pq$	$33pq$

We end this section with some examples.

Example 12. *Let* $F=F[2,7]$ *be a lattice with* 308 *atoms and* 452 *chemical bonds. Then one can see that*

$$M_1(F)=2672,\ M_2(F)=3948,\ M_2^*(F)=52.44\ and\ M_3(F)=40.$$

Example 13. *Let* $L=L[2,7]$ *be a nanotube with* 308 *atoms and* 462 *chemical bonds. Then one can see that* $\chi(L)=154$ *and* $X(L)=188.611$.

Example 14. *Let* $F=F[2,6]$ *be a nanotube with* 330 *atoms and* 480 *chemical bonds. Then one can see that* $ABC(F)=258.951$.

Example 15. *Let* $K = K[2,6]$ *be a nanotube with* 264 *atoms and* 384 *chemical bonds. Then one can see that* $GA(K) = 257.456$.

CONCLUSIONS

Among topological descriptors, topological indices are very important and they have a prominent role in chemistry. We have mentioned here some theoretical results about the Zagreb and conectivity indices of linear $[n]$-Pentacene, vertical and horizontal Pentacenic nanotube and nanotori.

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