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The Edge Version of Degree Based Topological Indices of $HAC_5C_6C_7[p, q]$ Nanotube

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Abstract. Let G be a simple molecular graph with vertex set $V(G)$ and edge set $E(G)$ respectively. The degree $deg(v)$ of the vertex $v \in V(G)$ is the number of vertices adjacent with vertex v. A graph can be recognized by a numeric number, a polynomial, a sequence of numbers or a matrix. A topological index is a numeric quantity associated with a graph which characterize the topology of graph and is invariant under graph automorphism. Topological indices play important role in mathematical chemistry especially in the quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) studies. In this paper we compute the edge version of some important degree based topological indices like Augmented Zagreb Index, Hyper-Zagreb Index, Harmonic Index and Sum-Connectivity Index of $HAC_5C_6C_7[p, q]$ Nanotube.

Keywords: Augmented-Zagreb Index; Hyper-Zagreb Index; Harmonic Index; Sum-Connectivity Index; Nanotubes.

1 Introduction and preliminary results

Graph theory is a not so young branch of discrete mathematics. It is generally accepted that it started with *Leonhard Euler's* paper on the seven bridges of *Königsberg* published in 1736. It has received more attention after the first book on Graph Theory which published in 1936. Since Graph theory became one of the fastest expanding branched of mathematics. Graph theory has been accepted and appreciated in Physics as well as in Biology, but it played wide range role in Chemistry. It made contributions in Chemical documentation, Structural chemistry, Physical chemistry, Inorganic chemistry, Quantum chemistry, Organic chemistry, Chemical synthesis, Polymer chemistry, Medicinal chemistry, Genomics, DNA studies and of recent date proteomics.

A branch of mathematical chemistry is *Chemical graph theory* which relates with the nontrivial applications of graph theory for solving the molecular problems. Its pioneers are Alexandru Balaban, Ante Graovac, Ivan Gutman, Haruo Hosoya, Milan Randić and Nenad Trinajstić. Chemical graph theory use algebraic invariants to minimize the structure of a molecule into a single number which denotes the energy of molecule, structural fragments, molecular branching and electronic structures. These graph theoretic invariants are used to associate with physical observations calculated by experiments.

Let G be a molecular graph having vertex set $V(G)$ and edge set $E(G)$. Two vertices in G connected by an edge, are said to be *adjacent*. The number of vertices in G, adjacent to given vertex v in G is called the *degree* of this vertex denoted by $deg(v)$. A *molecular graph* is a graph representing the carbon-atom skeleton of an organic molecule. Thus, the vertices in a molecular graph represent the carbon atoms, and its edges the carbon-carbon bonds.

A graph can be recognized by a numeric number, a polynomial, a sequence of numbers or a matrix. A topological index is a numeric quantity associated with a graph which characterize the topology of graph and is invariant under graph automorphism. The topological indices are structural invariants based on modeling of chemical structures by molecular graphs. There are some major classes of topological indices such as distance based topological indices, degree based topological indices and counting related polynomials and indices of graphs. Among these classes degree based topological indices are of great importance and play a vital role in chemical graph theory and particularly in chemistry. In more precise way, a topological index $Top(G)$ of a graph, is a number with the property that for every graph H isomorphic to G, $Top(H) = Top(G)$. The most common use of mathematical invariants which are also known as graph theoretical indices or topological indices are molecular descriptors in QSPR (Quantitative structure-property relationships) and QSAR (Quantitative structure-activity relationships).

The concept of topological indices came from Wiener while he was working on boiling point of paraffin, named this index as *path number*. Later on, the path number was renamed as *Wiener index* [28].

Let G be a graph. Then the Wiener index of G is defined as

$$W(G) = \frac{1}{2}\sum_{(u,v)} d(u,v) \tag{1}$$

where (u, v) is any ordered pair of vertices in G and $d(u, v)$ is $u - v$ geodesic. Here we define edge version of some important degree based topological indices.

1.1 Edge Version of Augmented Zagreb Index

Motivated by the success of the Atom bond connectivity index, *Furtula etal* [15] put forward its modified version named as *Augmented Zagreb Index*. The augmented Zagreb index possess the correlating ability among several topological indices. The edge version of Augmented Zagreb Index is defined as

$$_{e}AZI(G) = \sum_{ef\in E(L(G))} (\frac{deg_{L(G)}(e).deg_{L(G)}(f)}{deg_{L(G)}(e) + deg_{L(G)}(f) - 2})^3 \tag{2}$$

Preliminary studies indicate that Augmented Zagreb Index has an even better correlation potential than Atom bond connectivity index [17].

1.2 Edge Version of Hyper-Zagreb Index

G.H Shirdel, H. Rezapour and A.M. Sayadi introduced a new version of Zagreb index named Hyper-Zagreb index [22]. The edge version of Hyper-Index is defined as

$$_{e}HM(G) = \sum_{ef\in E(L(G))} \left(deg_{L(G)}(e) + deg_{L(G)}(f)\right)^2 \tag{3}$$

1.3 Edge Version of Harmonic Index

In 1980 Siemion Fajtlowicz created a computer program for automatic generation of conjectures in graph theory. Then he examined the possible relations between countless graph invariants, among which there was a vertex-degree-based quantity [14]. But this quantity did not attract any attention. In 2012 Zhang [30, 31] re-introduced this quantity and called it *Harmonic index* which is defined as [17]

$$_{e}H(G) = \sum_{ef\in E(L(G))} \frac{2}{deg_{L(G)}(e) + deg_{L(G)}(f)} \tag{4}$$

1.4 Edge Version of Sum-connectivity Index

Sum-connectivity index was proposed by Bo Zhou and Nenad Trinajstic [34]. They noticed that in the definition of Randić's branching index there is no a solid reason for using the product $deg(u) \times deg(v)$ of vertex degrees and this term may be replaced by the sum $deg(u) + deg(v)$ and we get *Sum-connectivity index*. The edge version of *Sum-connectivity index* is defined as

$$_{e}SCI(G) = \sum_{ef\in E(L(G))} \frac{1}{\sqrt{deg_{L(G)}(e) + deg_{L(G)}(f)}} \tag{5}$$

In view of above equation the original Randić' index is sometimes referred to as the *Product-connectivity index* [17].

2 Main results

The *carbon nanotubes* shows remarkable mechanical properties. Experimental studies have shown that they belong to the stiffest and elastic known materials. Diudea was the first chemist who consider the problem of topological indices of nano-structures.

In this paper we continue this program and compute the augmented Zagreb index, hyper-Zagreb index, harmonic index, sum-connectivity index of line graphs of $HAC_5C_6C_7[p,q]$ Nanotube.

$HAC_5C_6C_7[p,q]$ shown in Fig.1 is constructed by alternating C_5, C_6 and C_7 carbon cycles. It is tube shaped material but we consider it in the form of sheet shown in Fig.2. The two dimensional lattice of $HAC_5C_6C_7[p,q]$ consists of p rows and q periods. Here p denotes the number of pentagons in one row and q is the number of periods in whole lattice. A period consist of three rows.

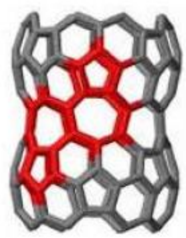

Fig. 1. $HAC_5C_6C_7[p,q]$ Nanotube

We now compute the edge version of augmented Zagreb index, hyper-Zagreb index, harmonic index and sum-connectivity index of $HAC_5C_6C_7[p,q]$ Nanotube with p columns and q rows. Throughout this figure we consider $p \geq 1$ and $q = 2$. The line graph of $HAC_5C_6C_7[p,q]$ nanotube shown in Fig.3 has $88p - 12$ edges with degree vertices 2, 3 and 4. The first edge partition has 2 edges with $d_{L(G)}(e) = d_{L(G)}(f) = 2$, the second edge partition has 12 edges with $d_{L(G)}(e) = 2$ and $d_{L(G)}(f) = 3$, the third edge partition has $6p+1$ edges with $d_{L(G)}(e) = d_{L(G)}(f) = 3$, the fourth edge partition has $12p + 10$ edges with $d_{L(G)}(e) = 3$ and $d_{L(G)}(f) = 4$ and the fifth edge partition has $70p - 37$ edges with $d_{L(G)}(e) = d_{L(G)}(f) = 4$.

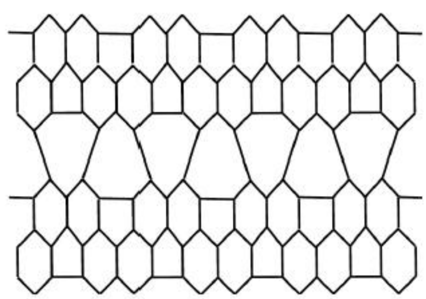

Fig. 2. $HAC_5C_6C_7[p,q]$ nanotube for $p = 4$ and $q = 2$.

Theorem 2.0.1. *For every $p \geq 1$ and $q = 2$, consider the graph of $G \cong HAC_5C_6C_7[p,q]$ nanotube. Then the ${}_eAZI(G)$ is equal to*

$${}_eAZI(G) = \frac{168657029}{108000}p - \frac{19007957}{43200}$$

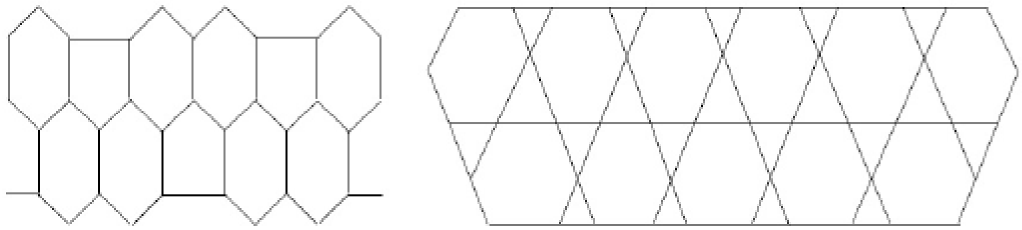

Fig. 3. $HAC_5C_6C_7$ and $L(HAC_5C_6C_7)$

Proof. Let G be the graph of $HAC_5C_6C_7[p,q]$ nanotube. Since from (2) we have

$$_eAZI(G) = \sum_{ef\in E(L(G))} \left(\frac{deg_{L(G)}(e).deg_{L(G)}(f)}{deg_{L(G)}(e)+deg_{L(G)}(f)-2}\right)^3$$

By using edge partition from Table.1, we get

$$_eAZI(G) = 2\times(\tfrac{2\times2}{2+2-2})^3 + 12\times(\tfrac{2\times3}{2+3-2})^3 + (6p+1)\times(\tfrac{3\times3}{3+3-2})^3 + (12p+10)\times(\tfrac{3\times4}{3+4-2})^3 + (70p-37)\times(\tfrac{4\times4}{4+4-2})^3$$

After doing some calculations, we get

$$_eAZI(G) = (\frac{2187}{32}+\frac{20736}{125}+\frac{35840}{27})p + \frac{729}{64}+\frac{3456}{25}-\frac{18944}{27}+112$$

After more simplification, we get

$$\Longrightarrow_e AZI(G) = \frac{168657029}{108000}p - \frac{19007957}{43200}$$

Theorem 2.0.2. *For every $p\geq 1$ and $q=2$, consider the graph of $G\cong HAC_5C_6C_7[p,q]$ nanotube. Then the $_eHM(G)$ is equal to*

$$_eHM(G) = 5284p - 1510$$

Proof. Let G be the graph of $HAC_5C_6C_7[p,q]$ nanotube. Since from (3) we have

$$_eHM(G) = \sum_{ef\in E(L(G))} \left(deg_{L(G)}(e)+deg_{L(G)}(f)\right)^2$$

By using edge partition from Table.1, we get

$$_eHM(G) = 2\times(2+2)^2 + 12\times(2+3)^2 + (6p+1)\times(3+3)^2 + (12p+10)\times(3+4)^2 + (70p-37)\times(4+4)^2$$

After doing some calculations, we get

$$\Longrightarrow_e HM(G) = 5284p - 1510$$

Theorem 2.0.3. *For every $p\geq 1$ and $q=2$, consider the graph of $G\cong HAC_5C_6C_7[p,q]$ nanotube. Then the $_eH(G)$ is equal to*

$$_eH(G) = \frac{321}{14}p - \frac{109}{420}$$

Proof. Let G be the graph of $HAC_5C_6C_7[p,q]$ nanotube. Since from (4) we have

$$_eH(G) = \sum_{ef\in E(L(G))} \frac{2}{deg_{L(G)}(e)+deg_{L(G)}(f)}$$

$(deg(e), deg(f))$ where $ef \in E(L(G))$	Number of edges
$(2,2)$	2
$(2,3)$	12
$(3,3)$	$(6p+1)$
$(3,4)$	$(12p+10)$
$(4,4)$	$(70p-37)$

Table 1. Edge partition of $L(HAC_5C_6C_7[p,q])$ based on degrees of end vertices of each edge.

By using edge partition from Table.1, we get

$_eH(G) = 2 \times \frac{2}{2+2} + 12 \times \frac{2}{2+3} + (6p+1) \times \frac{2}{3+3} + (12p+10) \times \frac{2}{3+4} + (70p-37) \times \frac{2}{4+4}$

After doing some calculations, we get

$$_eH(G) = (\frac{24}{7} + \frac{35}{2} + 2)p + \frac{24}{5} + \frac{1}{3} + \frac{20}{7} - \frac{37}{4} + 1$$

After more simplification, we get

$$\Longrightarrow_e H(G) = \frac{321}{14}p - \frac{109}{420}$$

Theorem 2.0.4. *For every $p \geq 1$ and $q = 2$, consider the graph of $G \cong HAC_5C_6C_7[p,q]$ nanotube. Then the $_eSCI(G)$ is equal to*

$$_eSCI(G) = (\frac{12}{\sqrt{7}} + \frac{35}{\sqrt{2}} + \sqrt{6})p + \frac{12}{\sqrt{5}} + \frac{1}{\sqrt{6}} + \frac{10}{\sqrt{7}} - \frac{37}{\sqrt{8}} + 1$$

Proof. Let G be the graph of $HAC_5C_6C_7[p,q]$ nanotube. Since from (5) we have

$$_eSCI(G) = \sum_{ef \in E(L(G))} \frac{1}{\sqrt{deg_{L(G)}(e) + deg_{L(G)}(f)}}$$

By using edge partition from Table.1, we get

$_eSCI(G) = 2 \times \frac{1}{\sqrt{2+2}} + 12 \times \frac{1}{\sqrt{2+3}} + (6p+1) \times \frac{1}{\sqrt{3+3}} + (12p+10) \times \frac{1}{\sqrt{3+4}} + (70p-37) \times \frac{1}{\sqrt{4+4}}$

After doing some calculations, we get

$$\Longrightarrow_e SCI(G) = (\frac{12}{\sqrt{7}} + \frac{35}{\sqrt{2}} + \sqrt{6})p + \frac{12}{\sqrt{5}} + \frac{1}{\sqrt{6}} + \frac{10}{\sqrt{7}} - \frac{37}{\sqrt{8}} + 1$$

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