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The Edge Version of Degree Based Topological Indices of NA_q^p Nanotube

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Abstract

Chemical graph theory is an important branch of mathematical chemistry which has wide range applications. In chemical graph theory a molecular graph can be recognized by a numerical quantity which is called a Topological index. Topological indices have some major classes but among these classes degree based topological indices have prominent role in chemical graph theory. 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 NA_q^p Nanotube.

Keywords

Augmented Zagreb Index, Hyper-Zagreb Index, Harmonic Index, Sum-Connectivity Index, NA_q^p, Nanotube

1. Introduction and Preliminary Results

Graph theory is an important branch of mathematics which is started by *Leonhard Euler's* as early as 1736. A hundred year before an important contribution of *Kirchhoff* had been made for the analysis of electrical networks. Several properties of special types of graphs known as *trees* were discovered by *Cayley* and *Sylvester*. The first book on graph theory was published in 1936 which received more attention. After the Second World War, further books were published on graph theory. Since then graph theory became one of the fastest expanding branches of mathematics.

Graph theory has many applications in engineering and science such as chemical, civil, electrical and mechanical engineering, architecture, management and control, communication, operational research, sparse matrix technology, combinatorial optimisation, physics, biology and computer science. But in chemistry graph theory has wide range applications; it has very important contributions in chemical documentation, structural chemistry, physical chemistry, inorganic chemistry, quantum chemistry, organic chemistry, chemical synthesis, polymer chemistry, medicinal chemistry, genomics, DNA studies and recent date proteomics.

Chemical graph theory is very important branch of mathematical chemistry. Its pioneers are Alexandru Balaban, Ante Graovac, Ivan Gutman, Haruo Hosoya, Milan Randić and Nenad Trinajstić. In chemical graph theory we 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. Physical observations calculated by experiments are used to associate with these graphs theoretic invariants.

A graph G consists of a vertex set $V(G)$ and edge set $E(G)$. Two vertices of G connected by an edge, are said to be *adjacent*. The *Degree* of a vertex v is the number of vertices adjacent with vertex v which is denoted by $deg(v)$. The carbon-atom skeleton of an organic molecule is represented with a *molecular graph*. In molecular graph vertices represents the carbon atoms and edges represents the bonds between the carbon atoms.

A topological index is a structural descriptor which is derived from a molecular graph that represents an efficient way to express in a numerical form the molecular size, shape, cyclicity and branching. The topological indices of molecular graphs are widely used for establishing correlations between the structure of a molecular compound and its physico-chemical properties or biological activity. There are some major classes of topological indices such as distance based topological indices, degree based topological indices, eccentricity 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 [1].

The concept of topological indices was given by 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* [2].

Let G be a molecular 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 the distance between the vertex u and vertex v.

The first degree based topological index is *Randic index* which was given by Milan Randic in 1975 in his paper *On characterization of molecular branching [3]*. The Randic index for a molecular graph G is defined as

$$R_{-\frac{1}{2}}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{deg(u)deg(v)}} \tag{2}$$

In this article we compute the edge version some important degree based topological indices which are Augmented Zagreb Index, Hyper-Zagreb Index, Harmonic Index and Sum-Connectivity Index of NA_q^p Nanotube. Now we define the edge versions of Augmented Zagreb Index, Hyper-Zagreb Index, Harmonic Index and Sum-Connectivity Index.

1.1. Edge Version of Augmented Zagreb Index

Furtula et al. [4] [5] modify the Atom bond connectivity index and named as *Augmented Zagreb Index*. The correlating ability among several topological indices possess by Augmented zagreb index. The edge version of Augmented Zagreb Index is defined as

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

As compared to Atom bond connectivity index Augmented Zagreb Index has better correlation potential [6].

1.2. Edge Version of Hyper-Zagreb Index

The Hyper-zagreb index was introduced by G.H Shirdel, H. Rezapour and A.M. Sayadi [7] which is basically a new version of Zagreb index. The edge version of Hyper-Zagreb Index is defined as

$${}_eHM(G) = \sum_{ef \in E(L(G))} \left(deg_{L(G)}(e) + deg_{L(G)}(f) \right)^2 \tag{4}$$

1.3. Edge Version of Harmonic Index

Zhang [8] [9] introduced this index in 2012 and called it *Harmonic index*. The edge version of Harmonic index is defined as [6]

$${}_eH(G) = \sum_{ef \in E(L(G))} \frac{2}{deg_{L(G)}(e) + deg_{L(G)}(f)} \tag{5}$$

1.4. Edge Version of Sum-Connectivity Index

Bo Zhou and Nenad Trinajstic [10] introduced *Sum-connectivity index*. In the definition of Randić's branching index they replaced the product $deg(u) \times deg(v)$ of vertex degrees with the sum $deg(u) + deg(v)$ and get *Sum-connectivity index*. The edge version of *Sum-connectivity index* is defined as

$${}_eSCI(G) = \sum_{ef \in E(L(G))} \frac{1}{\sqrt{deg_{L(G)}(e) + deg_{L(G)}(f)}} \tag{6}$$

For future research and more history of these degree based topological indices "Augmented Zagreb, Hyper-Zagreb, Harmonic and Sum-Connectivity" readers can see the papers series [11]-[39].

2. Main Results

2.1 NA_q^p Nanotube

Carbon nanotubes are the allotropic forms of carbon with a cylindrical nano-structures. *Carbon nanotubes* form an interesting class of carbon nonmaterial. There are three types of nanotubes namely, armchair, chiral and zigzag structures nanotubes. These *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 some degree based topological indices of line graph of NA_q^p nanotube.

We consider the $q \times p$ quadrilateral section P_q^p with $q \geq 2$ hexagons on the top and bottom sides and $q \geq 2$ hexagons on the lateral sides cut from the regular hexagonal lattice *L*. If we identify two lateral sides of P_q^p such that we identify the vertices u_0^j and u_q^j, for $j = 0, 1, 2, \cdots, p$ then we obtain the nanotube NA_q^p shown in **Figure 1** [40]. Throughout in **Figure 2** we consider $p = q > 2$.

We now compute the edge version of augmented zagreb index, hyper-zagreb index, harmonic index and sum-connectivity index of NA_q^p nanotube. Throughout this figure we consider $p = q \geq 2$. The line graph of NA_q^p nanotube has $6p^2 + p + s + k - 5$ edges with degree vertices 2, 3 and 4. The first edge partition has *s* edges with $d_{L(G)}(e) = d_{L(G)}(f) = 2$ the second edge partition has $2p + 2$ edges with $d_{L(G)}(e) = 2$ and $d_{L(G)}(f) = 3$, the third edge partition has k edges with $d_{L(G)}(e) = 2$ and $d_{L(G)}(f) = 4$, the fourth edge partition has $4p - 6$ edges with $d_{L(G)}(e) = d_{L(G)}(f) = 3$, the fifth edge partition has $8p - 8$ edges with $d_{L(G)}(e) = 3$ and $d_{L(G)}(f) = 4$ and the sixth edge partition has $6p^2 - 13p + 7$ edges with $d_{L(G)}(e) = d_{L(G)}(f) = 4$.

2.2. Edge Version of Augmented Zagreb Index, Hyper-Zagreb Index, Harmonic Index and Sum-Connectivity Index of NA_q^p Nanotube

Theorem 2.2.1. For every $p = q \geq 2$, consider the graph of $G \cong NA_q^p$ nano-

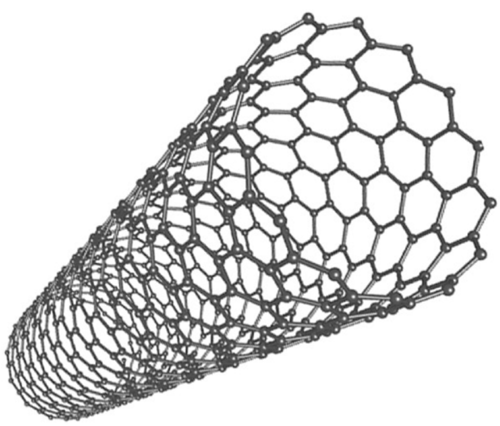

Figure 1. NA_q^p Nanotube.

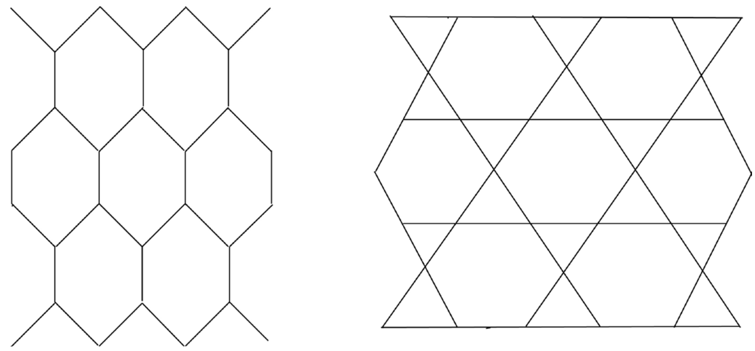

Figure 2. NA_q^p and $L\left(NA_q^p\right)$ for $p=q=3$.

tube. Then the ${}_eAZI\left(G\right)$ is equal to

$${}_eAZI\left(G\right)=\frac{3072}{27}p^2-\frac{4015657}{54000}p+8s+8k-\frac{3261061}{108000}$$

Proof. Let G be the graph of NA_q^p nanotube. Since from (3) we have

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

By using edge partition in Table 1, we get

$$\begin{aligned}{}_eAZI\left(G\right)&=s\times\left(\frac{2\times2}{2+2-2}\right)^3+\left(2p+2\right)\times\left(\frac{2\times3}{2+3-2}\right)^3+k\times\left(\frac{2\times4}{2+4-2}\right)^3\\&+\left(4p-6\right)\times\left(\frac{3\times3}{3+3-2}\right)^3+\left(8p-8\right)\times\left(\frac{3\times4}{3+4-2}\right)^3\\&+\left(6p^2-13p+7\right)\times\left(\frac{4\times4}{4+4-2}\right)^3\end{aligned}$$

After an easy simplification, we obtain

$$\begin{aligned}{}_eAZI\left(G\right)&=\frac{3072}{27}p^2+\left(\frac{2916}{64}+\frac{13824}{125}-\frac{6656}{27}+16\right)p\\&+8s+8k+\frac{3584}{27}-\frac{2187}{32}-\frac{13824}{125}+16\end{aligned}$$

After more simplification, we get

$$\Rightarrow {}_eAZI\left(G\right)=\frac{3072}{27}p^2-\frac{4015657}{54000}p+8s+8k-\frac{3261061}{108000}$$

Theorem 2.2.2. For every $p=q\ge2$, consider the graph of $G\cong NA_q^p$ nanotube. Then the ${}_eHM\left(G\right)$ is equal to

$${}_eHM\left(G\right)=384p^2-246p+16s+36k-110$$

Proof. Let G be the graph of NA_q^p nanotube. Since from (4) we have

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

By using edge partition in Table 1, we get

Table 1. Explanation of the terms present in **Table 2**.

Number of edges	Explanation
s	$s=2$ when $p\equiv 0(\mathrm{mod}\,2)$ and $s=0$ when $p\equiv 1(\mathrm{mod}\,2)$
k	$k=2$ when $p\equiv 0(\mathrm{mod}\,2)$ and $k=4$ when $p\equiv 1(\mathrm{mod}\,2)$

Table 2. Edge partition of $L\left(NA_q^p\right)$ based on degrees of end vertices of each edge.

$(deg(e),deg(f))$ where $ef\in E(L(G))$	Number of edges
$(2,2)$	s
$(2,3)$	$2p+2$
$(2,4)$	k
$(3,3)$	$4p-6$
$(3,4)$	$8p-8$
$(4,4)$	$6p^2-13p+7$

$$
{}_eHM(G)=s\times(2+2))^2+(2p+2)\times(2+3)^2+k\times(2+4)^2+(4p-6)\times(3+3)^2 \\
+(8p-8)\times(3+4)^2+\left(6p^2-13p+7\right)\times(4+4)^2
$$

After an easy simplification, we obtain

$$
\Rightarrow {}_eHM(G)=384p^2-246p+16s+36k-110
$$

Theorem 2.2.3. For every $p=q\geq 2$, consider the graph of $G\cong NA_q^p$ nanotube. Then the ${}_eH(G)$ is equal to

$$
{}_eH(G)=\frac{3}{2}p^2+\frac{491}{420}p+\frac{1}{2}s+\frac{1}{3}k-\frac{243}{140}
$$

Proof. Let G be the graph of NA_q^p nanotube. Since from (5) we have

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

By using edge partition in **Table 1**, we get

$$
{}_eH(G)=s\times\frac{2}{2+2}+(2p+2)\times\frac{2}{2+3}+k\times\frac{2}{2+4}+(4p-6)\times\frac{2}{3+3} \\
+(8p-8)\times\frac{2}{3+4}+\left(6p^2-13p+7\right)\times\frac{2}{4+4}
$$

After an easy simplification, we obtain

$$
{}_eH(G)=\frac{3}{2}p^2+\left(\frac{4}{5}+\frac{4}{3}+\frac{16}{7}-\frac{13}{4}\right)p+\frac{1}{2}s+\frac{1}{3}k+\frac{4}{5}-\frac{16}{7}+\frac{7}{2}-2
$$

After more simplification, we get

$$
\Rightarrow {}_eH(G)=\frac{3}{2}p^2+\frac{491}{420}p+\frac{1}{2}s+\frac{1}{3}k-\frac{243}{140}
$$

Theorem 2.2.4. For every $p=q\geq 2$, consider the graph of $G\cong NA_q^p$ nanotube. Then the ${}_eSCI(G)$ is equal to

$$ {}_{e}SCI(G)=\frac{6}{\sqrt{8}}p^{2}+\left(\frac{2}{\sqrt{5}}+\frac{4}{\sqrt{6}}+\frac{8}{\sqrt{7}}-\frac{13}{\sqrt{8}}\right)p+\frac{s}{2}+\frac{k}{\sqrt{6}}+\frac{2}{\sqrt{5}}-\frac{8}{\sqrt{7}}+\frac{7}{\sqrt{8}}-\sqrt{6} $$

Proof. Let G be the graph of NA_q^p nanotube. Since from (6) we have

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

By using edge partition from **Table 2**, we get

$$ {}_{e}SCI(G)=s\times\frac{1}{\sqrt{2+2}}+(2p+2)\times\frac{1}{\sqrt{2+3}}+k\times\frac{1}{\sqrt{2+4}}+(4p-6)\times\frac{1}{\sqrt{3+3}} $$
$$ +(8p-8)\times\frac{1}{\sqrt{3+4}}+\left(6p^{2}-13p+7\right)\times\frac{1}{\sqrt{4+4}} $$

After doing some calculations, we get

$$ \Rightarrow {}_{e}SCI(G)=\frac{6}{\sqrt{8}}p^{2}+\left(\frac{2}{\sqrt{5}}+\frac{4}{\sqrt{6}}+\frac{8}{\sqrt{7}}-\frac{13}{\sqrt{8}}\right)p+\frac{s}{2}+\frac{k}{\sqrt{6}}+\frac{2}{\sqrt{5}}-\frac{8}{\sqrt{7}}+\frac{7}{\sqrt{8}}-\sqrt{6} $$

3. Conclusion

In this paper, we have discussed the edge version of augmented zagreb index, hyper-zagreb index, harmonic index and sum-connectivity index. We have considered the line graph of NA_q^p nanotube and we have computed the edge version of augmented zagreb index, hyper-zagreb index, harmonic index and sum-connectivity index for NA_q^p nanotube.

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